Programmübersicht

Willkommen zur DGMS 2017

Die 50. Jahrestagung der Deutschen Gesellschaft für Massenspektrometrie (DGMS) wird vom 5. März bis zum 8. März 2017 in Kiel stattfinden. Als Gastgeber im Namen der Deutschen Gesellschaft für Massenspektrometrie begrüßen Sie in diesem Jahr Dr. Tassilo Muskat und Prof. Dr. Jürgen Grotemeyer von der Christian-Albrechts-Universität zu Kiel.

Veranstaltungsort

Hörsaalgebäude Olshausenstraße 75

(ehemals EWF)

Olshausenstraße 75

24118 Kiel

Freuen Sie sich am Sonntag auf interessante workshops, den Wolfgang Paul Vortrag von Brian Chait und ein gemeinsames Beisammensein im Anschluss.
Am Montag dürfen Sie sich auf an die 50 Vorträge, darunter zwei Plenarvorträge von Ron M. A. Heeren und von Valérie Gabelica, der Verleihung des Wolfgang-Paul-Studienpreises sowie über 75 Posterbeiträge freuen.
Am Dienstag können Sie neben der Preisverleihung des Mattauch-Herzog Förderpreises über 30 Vorträgen, darunter einen -inzwischen in guter Tradition- fachfremden Vortrag und einen Plenarvortrag von Richard A. J. O'Hair, sowie weiteren etwa 75 Posterbeitragen beiwohnen. Verpasssen Sie nicht die Mitgliederversammlung der DGMS und das Konferenzdinner an diesem Tag!
Abgerundet und abgeschlossen wird die Tagung am Mittwoch durch ein Programm, das die Verleihung des DGMS-Preises für die Massenspektrometrie in den Biowissenschaften und noch einmal 20 Vorträge, darunter einen Plenarvortrag von Andrej Shevchenko, enthält. Gegen 13 Uhr dürfen wir Ihnen dann eine gute Heimreise wünschen und übergeben den Staffelstab an das nächste Team.

VORTRÄGE

Vortragende werden gebeten, ihre Präsentation morgens bis 8:15 Uhr im Tagungsbüro abzugeben. Vorträge sollten als Powerpoint (mit eingebetteter Schriftart, ppsx oder pps File) oder als PDF File abgegeben werden. Die Benutzung eines eigenen Rechners für den Vortrag ist in keinem Fall möglich. Bitte stellen Sie sich vor der Sitzung bei Ihrer Sitzungsleitung vor.

POSTERSESSION

Die Postersession findet in der Eingangshalle der ehemaligen EWF statt. Poster mit ungeraden Nummern werden am Montag in der Zeit von 18:00 – 20:30 Uhr, Poster mit geraden Nummern am Dienstag von 16:30 – 18:30 Uhr präsentiert.
Während der Postersession am Montagabend gibt es verschiedene Getränke und Fingerfood. Dazu bietet die Fa. Bruker Daltonik einen Cocktailstand an, der sich vor den Hörsälen befindet. Zur Postersession am Dienstag gibt es verschiedene Getränke sowie kleine Snacks, die die Fa. Agilent freundlicherweise bereitstellt.

WLAN

Im Tagungsgebäude existiert ein WLAN – Netz, in das Sie sich einloggen können. Sie benötigen dazu einen Anmeldecode und ein Password, die Sie in Ihren Unterlagen finden, bzw. im Tagungsbüro erhalten können. Sollte Ihre Hochschule am „eduroam“ teilnehmen, erhalten Sie auch über diese Möglichkeit Zugang zum Internet.

Conference4me-App

Mit der App Conference4me haben Sie jederzeit Zugriff auf das gesamte Tagungsprogramm inklusive aller Vorträge, Sessions und Abstracts. Sie können nach bestimmten Themen oder Autoren sich bequem ihr persönliches Programm zusammenstellen. Die App ist kostenfrei und für alle gängigen Mobilplattformen verfügbar.

Conference4me für Android
Conference4me für iOS
Conference4me für Windows Phone
Conference4me für kindle fire

Um Zugriff auf das Tagungsprogramm zu erhalten, fügen Sie bitte nach der Installation DGMS 2017 zu Ihren Konferenzen hinzu.

MITGLIEDERVERSAMMLUNG

Die Mitgliederversammlung findet am Dienstag um 15:45 Uhr im Anschluss an den Plenarvortrag im Hörsaal 3 statt. Bitte tragen Sie sich in die ausliegenden Teilnehmerlisten ein.

GARDEROBE

Sie finden eine Garderobe im Seminarraum 24. Bitte beachten Sie, dass für Ihre Garderobe oder Gepäck keine Haftung übernommen wird.

Eröffnungsabend:

Nach dem Wolfgang-Paul-Vortrag laden wir Sie zu einem "getting together" im Erdgeschoss des Gebäudes Olshausenstraße 75 ein. Sie finden warme und kalte Speisen an insgesamt drei Standorten. Wir danken der Firma ThermoFisher Scientific für die freundliche Unterstützung des catering.

KONFERENZDINNER

Das Konferenzdinner findet am Dienstag, dem 7. März ab 19:30 Uhr im Fuego del Sur (An der Halle 400 1) statt. Der Eingang befindet sich am Gebäude rechts.
Es erwartet Sie ein Buffet inklusive Getränke bis ca. 23:30 Uhr. Anschließend können Sie gern auf Selbstzahlerbasis im Fuego del Sur verbleiben. Das Restaurant schließt um 0:30 Uhr. Kostenpflichtige Parkplätze sind in ausreichender Menge vorhanden. Das Restaurant ist leicht zu Fuß entlang der Förde von den meisten Hotels zu erreichen (Typisch 10 – 20 min Fußweg).

Impressum

Inhaltlich verantwortlich:

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Dr. Tassilo Muskat

Institut für Physikalische Chemie
Christian-Albrechts-Universität zu Kiel
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Layout:

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Bilder der Titelseite:
Prof. Dr. Jürgen Grotemeyer

Logo:
Björn Raupers

Für die großzügige Unterstützung der Tagung danken wir

Agilent Technologies

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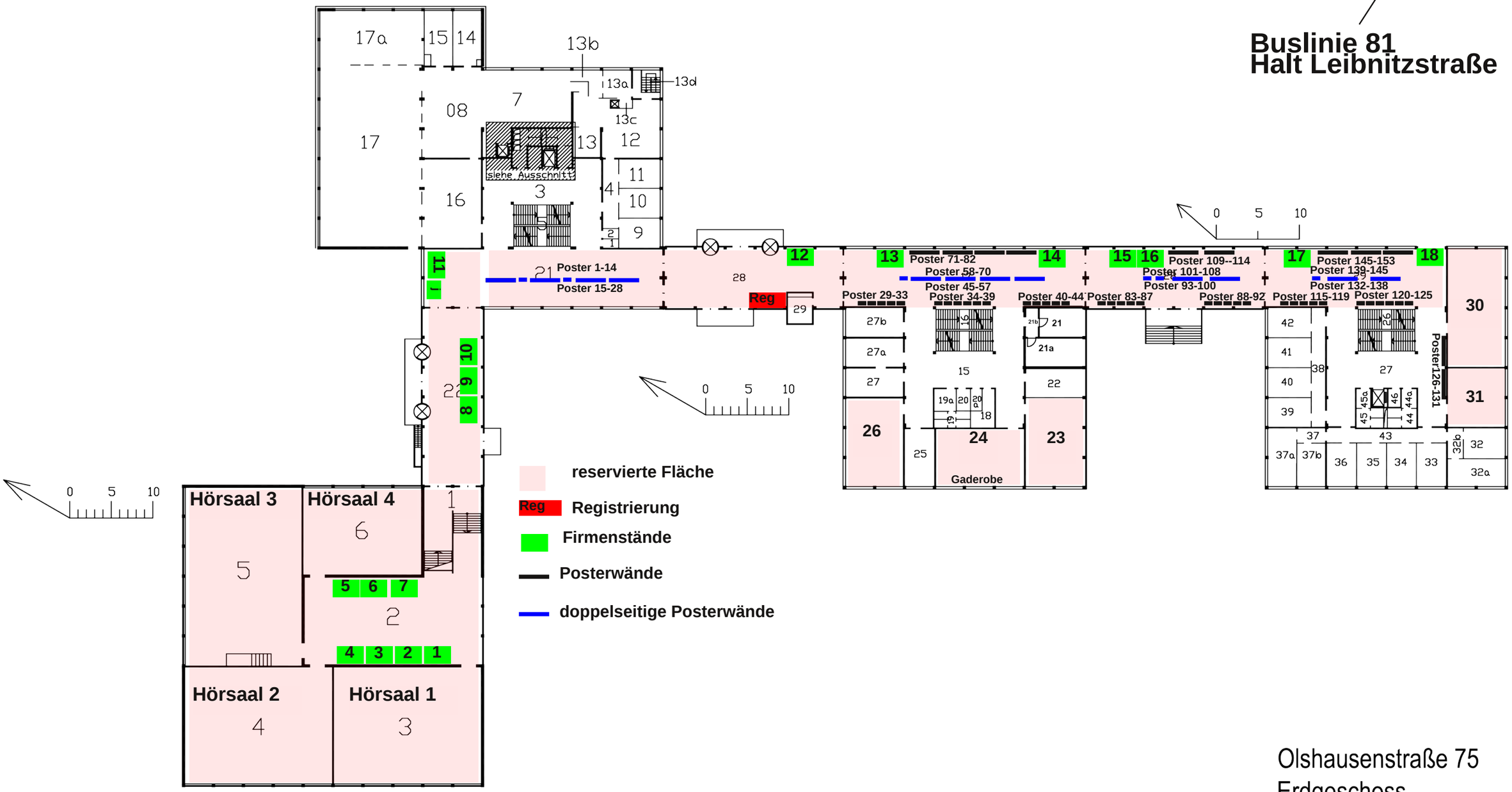
Buslinie 61/62
Halt: Bremerskamp

Buslinie 61/62
Halt Leibnitzstraße

Olshausenstraße

Buslinie 81
Halt Leibnitzstraße



Olshausenstraße 75
Erdgeschoss

Stand 1 - Thermo Fisher Scientific

Thermo Fisher Scientific Inc. is the world leader in serving science, with revenues of $17 billion and more than 50,000 employees in 50 countries. Our mission is to enable our customers to make the world healthier, cleaner and safer. We help our customers accelerate life sciences research, solve complex analytical challenges, improve patient diagnostics and increase laboratory productivity. Through our premier brands - Thermo Scientific, Applied Biosystems, Invitrogen, Fisher Scientific and Unity Lab Services - we offer an unmatched combination of innovative technologies, purchasing convenience and comprehensive support. For more information, please visit www.thermofisher.com.

Stand 2 - Agilent

Agilent is a leader in Pharmaceutical, Life Sciences, Diagnostics, and applied markets. The company provides laboratories worldwide with instruments, services, consumables, applications and expertise, enabling customers to gain the insights they seek. Agilent has about 12500 employees globally and had revenues of $4.2 billion in fiscal year 2016. The comprehensive and trusted portfolio offers the most powerful and reliable solutions for diverse application areas. Backed by the technology leading "Cary" brand, as well as Agilent's world-wide service and support organization, Agilent provides a full range of solutions from routine to research.

Stand 3 - Bruker Daltonics

Bruker Daltonik GmbH provides a broad range of high performance, easy to use Mass Spectrometry (MS) and analytical separation systems. Bruker delivers a series of innovative, fully integrated systems for use in the Pharmaceutical, Life Science, Applied Analytical, and Clinical Research areas. Utilizing a product and technology portfolio which includes MALDI-TOF MS, ESI-TOF and qTOF MS, Ion Trap MS, FTMS and triple-quad systems, Bruker provides the best solutions for the very latest analytical questions.

Stand 4 - Shimadzu Deutschland GmbH

1875 gegründet, ist Shimadzu heute ein weltweit führender Hersteller von Systemen der Instrumentellen Analytik für Industrie und Wissenschaft. Die Geräte dienen der Produktsicherheit, dem Umwelt- und Verbraucherschutz. Sie entsprechen den internationalen Standards und werden in nahezu allen Fertigungsindustrien eingesetzt, im Gesundheitswesen sowie in der Lebensmittelherstellung, -verarbeitung und -sicherheit. Sie werden für Routine- und HighEnd-Anwendungen genutzt, für Prozess und QualitÃ¤tskontrolle sowie Forschung und Entwicklung. Niederlassungenin 76 Ländern und etwa 10.000 Mitarbeiter gewährleisten die Kundennähe.

Shimadzu Deutschland GmbH bedient den deutschen Markt mit Beratungs- und Produktlösungen sowie Serviceleistungen für Massenspektrometrie, Chromatographie (LC-MS/MS, HPLC, GC-MS/MS, GC), Life Sciences (Maldi, Accuspot,ChiP), Spektroskopie (UV-Vis, FT-IR, AAS), Summenparameter (TOC) sowie für Geräte in der Materialprüfung. Die LabSolution Softwarefamilie integriert Chromato- und non-Chromato- Geräte in einer Client/Server Umgebung. Neben seiner Vertriebszentrale in Duisburg unterhält Shimadzu Deutschland sechs Technische Büros und Service-Stützpunkte in regionalen Einzugsgebieten und gewährleistet damit schnelle und kurze Wege zu den Kunden.

Stand 5 - Leybold GmbH

Leybold bietet Vakuumlösungen für ein breites Spektrum moderner Produktions- und Analyseverfahren sowie für Forschungszwecke an.
Die Entwicklung von Systemen zur Vakuumerzeugung und Prozessgasförderung stellt die Kernkompetenz des Unternehmens dar.

Stand 6 - AB SCIEX Germany GmbH

Stand 7 - Waters GmbH

Stand 8 - KR Analytical Ltd.

Stand 9- MS Vision

MS Vision provides excellent, cost-effective, multi-vendor LC-MS service throughout Europe, performed by a team of senior OEM-trained, highly experienced mass spectrometry specialists. We are dedicated to high quality field service, hence we excel both in direct communication, quality of engineering, parts availability in order to achieve maximum uptime of your instrumentation. Operated via our logistics center, we provide multi-lingual call handling, technical helpdesk and overnight shipment of parts. For our contract customers we offer exchange programs for rotary vane and turbo-molecular pumps as well as electronics components. We support the LC-MS product range from Waters corporation, Sciex and Thermo Scientific, including a broad range of associated (U)HPLC systems. Beside service we have developed a niche market product, in close collaboration with experst in the academic field. Our High Mass Q-Tof has set the standard for Native Mass Spectrometry applications. Also we market a range of pre-owned instruments, which come fully refurbished, including installation and warranty. Our current stock comprises an Orbitrap Velos, XEVO Q-Tof, API 5500 Q-Trap, API 4000 Q-Trap, TSQ Vantage, Quattro Premier XE

Stand 10 - SunChrom GmbH

SunChrom GmbH is a midsize company located in the Rhein-Main-Area near Frankfurt am Main in Germany. Funded almost 30 years ago, SunChrom has specialised on the development and marketing of HPLC system solutions for beverage analytics as well as front-end applications and sample preparation systems for mass spectrometry, in particular for MALDI-MS Imaging.

The instrumentation provided by SunChrom covers the entire sample preparation for the MALDI-MSI. The product portfolio includes the MALDI-Sprayer SunCollect, that can be used for matrix and enzyme application as well as the incubation chamber SunDigest, that allows fully-controlled and absolutely reproducible on-tissue digestion of proteins.

Stand ? - JEOL (Germany) GmbH

JEOL offers systems for microscopic imaging with resolutions spanning to the atomic range, and systems for the analysis of chemical compositions in the micro- and nanoscale. The JEOL clientele includes universities and research institutes as well as companies of different size and industrial sectors.

With extensive knowledge and experience in electron optics and both mass and NMR spectrometry for decades, JEOL is your reliable partner not only for biological and medical research but also for the development, characterization and quality control of materials.

Stand 11 - PerkinElmer

For People, For the Planet,
For the Better

The challenges we face today have never been greater. Our mission is to help you detect environmental threats, ensure food quality and safety, diagnose and treat disease earlier, develop drugs and therapies faster and analyze information to unlock new insights for a better tomorrow.

Our solutions in the areas of Diagnostics, Life Sciences, and Applied Markets help scientists, lab professionals, and clinicians answer important questions needed to help customers gain earlier and more accurate insights.

We bring together important technologies such as detection, imaging, informatics, and key services to help scientists and clinicians address some of the most daunting scientific challenges today. These professionals need to measure, analyze, visualize, and report information, relying on some of the most advanced technologies and expertise to gain the greatest insights required to improve lives and the world around us.

Mass spectrometry is a growing technique and market, and one in which PerkinElmer invests significantly. At the Annual Meeting of the DGMS PerkinElmer will introduce its latest innovation in mass spectrometry, the QSight Triple Quadrupole LC/MS/MS. It delivers the key technologies you count on in a triple quadrupole end-to-end, compact and easy-to-use-solution. Its unique StayClean-technology hot-surface induced desolvation (HSID™), a multi-orthogonal sampling interface can significantly increase your uptime. Ions are transferred from the HSID interface to the system's Laminar Flow Ion Guide™, then moved to the analyzing region by a flow of background gas – no axial electrical fields are necessary. This means the system is not susceptible to field fluctuations and delivers consistently high levels of sensitivity, resolution and performance.

Stand 12 - Advion

Mass Spec Solutions for Chemical Biology

Advion is the partner of choice for biopharmaceutical, academic/government researchers, and industrial chemists seeking to enhance their chemical synthesis knowledge, workflow and mass spectrometry results. Using our deep scientific and engineering expertise, we develop a broad portfolio of chemist-centric, purpose-built mass spectrometers, nanoelectrospray ionization sources, flow-chemistry synthesis systems and consumables characterized by their reliability, high quality and flexibility.

Stand 13 - Merck

Gegründet 1668 ist Merck mit Sitz in Darmstadt die älteste pharmazeutische und chemische Firma der Welt. Das analytische Portfolio von Merck wurde durch die Aquisition von Sigma-Aldrich (incl. der Marke Supelco) signifikant erweitert, und beinhaltet für LC-MS Anwendungen u.a. Produkte für die Probenvorbereitung, Chromatographiesäulen und -zubehör, Reagenzien, Standards & Referenzmaterialien. Die speziellen Lösungsmittel und Puffer für die MS haben in der Regel LC/MS-relevante Spezifikationen, wie z.B. ein bestimmtes Signal/Rauschverhältnis einer Marker-Verbindung. Ein großer Teil der HPLC-Säulen sind LC-MS-geeignet und dafür entwickelt worden. Zu den bekannten Säulenfamilien gehören u.a. ZIC-HILIC, Purospher STAR, Chromolith (monolithische Säulen), Ascentis Express & BIOshell (Fused Core) Säulen. Zahlreiche Methoden und Applikationen aus den verschiedensten Analytbereichen wie z.B. Biomarker, pharmazeutische Verbindungen, Proteine & Peptide, Pestizide sind mit diesen Säulen entwickelt worden und online unter www.sigma-aldrich.com verfügbar. Insgesamt bietet Merck ein umfassendes Portfolio für LC-MS-Anwendungen an, das den gesamten Arbeitsfluß von Probenvorbereitung über Trennung bis hin zur Kalibration abdeckt. Des Weiteren erhalten Sie auch Unterstützung bei Ihrer Methodenentwicklung durch technische Beratung.

Stand 14 - Restek GmbH

Chromatografie ist unser Geschäft - das macht uns stark
Die Restek GmbH bietet deutschlandweit Säulen, Zubehör und Verbrauchsmaterialien von Restek® für die bestmögli-che Chromatografie an. Von der Probenahme und –aufgabe über die Trennung bis hin zur Qualitätskontrolle liefert die Restek GmbH nicht nur einzelne Produkte, sondern komplette Lösungen auf der Basis von Restek entwickelten Technologien.
30 Jahre Erfahrung in der Chromatografie
Die Entwicklung und Weiterentwicklung der Technologien macht die Restek GmbH zu einer wertvollen Wissensquel-le. In ganz Deutschland betreuen die Mitarbeiter Fachleute aus der industriellen Chemie, Biotechnologie, Lebens-mittelchemie, Umweltchemie und vielen anderen Bereichen.
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Kompetente Kundenberater stehen Ihnen ständig zur Verfügung. Ein breit gefächertes Wissen und ständige Weiterbildung sind Grundlage, um Ihre Fragen auf Augenhöhe mit Ihnen zu diskutie-ren. Auf Fachkongressen und Ausstellungen werden Sie immer Restek Berater finden. Nutzen Sie diese wertvolle Wissensquelle.
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Um Sie zu informieren nutzen wir die gesamte Bandbreite der Kommunikation. Homepage, Literatur, Applikationen, Newsletter, Seminare und persönliche Ansprache stehen Ihnen uneingeschränkt zur Seite.

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Stand 15 - MasCom Technologies

MasCom Technologies refurbishes and sells mass spectrometer from Thermo Fisher. MasCom provides worldwide service and repair for ion trap MS systems, quadrupole MS systems and high resolution GC-MS systems from Thermo Fisher. MasCom also stocks spare parts and consumables for these instruments, which are available through MasCom's on-line shop at www.mascom-bremen.de. Almost exclusively MasCom offers this service for the MAT95XL/XP instruments for more than 20 years. We provide telephone support as well as a repair service for electronic boards or mechanical parts of the mass spectrometer. In addition we offer repair of roughing and turbo molecular pumps which are used on the mass spectrometers. We have sold many used mass spectrometer over the past years and already 3 MAT95 XL/XP systems this year.
MasCom offers full service or maintenance contracts with reaction times (depending on the location) of faster than 24 hours. MasCom's service is highly qualified documented such that Thermo Fisher uses MasCom as one of 'their engineers' for servicing the actual model (DFS) of the high resolution GC-MS system.
Most recently, we have introduced our GC-APPI interface for all OrbitrapTM and ExactiveTM LCMS systems. This interface enables the user to run GCMS experiments on his LCMS instrument without sacrificing the high resolution and accurate mass capabilities.

Stand 16- SERVA Electrohoresis GmbH

SERVA Electrophoresis GmbH – Heidelberg SERVA offers products of highest quality since 1953 to customers in industry and academic research departments. The main business areas include development and marketing of reagents for electrophoresis as well as selling fine and biochemical like albumin, antibiotics, detergents, enzymes, enzyme substrates, inhibitors, dyes, buffer substances and ion exchange media. As an important supplier in the area of protein electrophoresis SERVA offers numerous reagents like dyes for labelling and detection, buffer and gel solutions, protein size

standards, pI standards, chemiluminescence kits for Western Blotting, and more. In Heidelberg SERVA develops and produces a broad choice of ready-made gels, in particular SERVALYTTM PRECOTESTM and FocusGel for isoelectric focusing of proteins and SERVAGel™ PRiME mini vertical gels for die SDS PAGE (1D, 2D) or native PAGE, also for Blue Native PAGE in the format of 10 x 10 cm. For 2D Gel electrophoresis SERVA produces IPG-Strips for the first dimension in lengths from 7 to 24 cm, as well as large format horizontal 2D gels (25.5 x 20 cm and 25 x 11 cm) under the seal of quality „High Performance Electrophoresis“ (HPETM) for the HPETM-Tower-Gel system for high resolution electrophoresis in the second dimension. The SERVA ICPLTM-Kit (ICPL = Isotope-coded Protein Labelling), under inclusion of the software ICPLQuant, enables mass-spectrometrical quantification of proteins for the differential expression analysis of up to four different cell conditions, Trypsin MS approved as high specific and very stable endoprotease for protein digestion in MS analysis. In addition to the reagents SERVA supplies high value electrophoresis equipment like flatbed and vertical chambers, power supplies, scanner and camera systems for gel documentation and image analysis. SERVA Electrophoresis GmbH is a medium sized, international oriented company in the Life Science industry located in Heidelberg, Germany.

Stand 17 - Biosolve

We produce and distribute selected high purity solvents and chemicals for research, routine laboratories and industries .In addition to serving the traditional chemical field with analytical, chemically pure and pharmaceutical grades of chemicals and solvents, we have developed several spcialty lines such as: HPLC, LC-MS & ULC/MS grades solvents and formulations for liquid chromatography Solvents for organic trace analysis and environmental analysis: LV-GC, Dioxins, Furans & PCB,s grades Peptide synthesis grade solvents and chemicals Ancillary reagents and formulations for DNA & RNA synthesis Chemicals, dyes, buffers and transfection kits for Molecular Biology Solvents and formulations for the electronic industry Synthetic lipids for the pharmaceutical industry and R&D use.

Stand 18 - ERC GmbH

Seit über 35 Jahren liefern wir hochwertige analytische Geräte und Systeme europaweit an renommierte kleine und große Unternehmen, im Bereich der Forschung bis hin zur Qualitätskontrolle.
In Deutschland waren wir die Ersten, die Degasser und die Brechungsindex-Messung in der analytischen HPLC eingeführt haben. 2005 brachten wir ein Gerät mit neuer Charged Aerosol Detektionstechnologie, der ersten neuen Technologie in der HPLC seit 20 Jahren, sehr erfolgreich auf den Markt. Auch heute sind wir in vielem Pioniere, wenn es gilt, neue Techniken und Methoden in den Markt einzuführen und exklusiv anzubieten.

Sie finden bei uns Produkte für LC/MS, HPLC/UHPLC, CCC, SMBC, SFE und die Massenspektrometrie.

50. Jahrestagung der Deutschen Gesellschaft für Massenspektrometrie

Datum: Sonntag, 05.03.2017

11:00 - 18:00	**So_Tag: Tagungsbüro**
13:00 - 15:00 **Seminarraum 30**	**WS 1a: Data processing in mass spectrometry imaging** Chair der Sitzung: **Bernhard Spengler** Chair der Sitzung: **Andreas Römpp** Andreas Römpp and Bernhard Spengler
13:00 - 15:00 **Seminarraum 26**	**WS 2a: Workshop "Core Facilities"** Chair der Sitzung: **Christof Lenz** Chair der Sitzung: **Sabine Metzger** Chair der Sitzung: **Axel Imhof** Christof Lenz, Universitäsmedizin Göttingen; Axel Imhof, Ludwig-Maximilians-Universität München
13:00 - 15:00 **Hörsaal 4**	**WS 3a: Lipidomics: A Workshop about Lipid Function and Analysis** Chair der Sitzung: **Robert Ahrends** Chair der Sitzung: **Dominik Schwudke** Chair der Sitzung: **Cristina Coman** Chair der Sitzung: **Andrej Shevchenko** Dominik Kopcynski,
13:00 - 15:00 **Seminarraum 31**	**WS 4a: Wissenschaftliches Publizieren** Chair der Sitzung: **Jürgen Gross** Chair der Sitzung: **Jürgen Grotemeyer**
14:00 - 15:00 **Hörsaal 2**	**WS 5a: Grundlagen der Massenspektrometrie** Chair der Sitzung: **Dietmar Kuck** Chair der Sitzung: **Matthias Letzel** Chair der Sitzung: **Mathias Schäfer**
15:00 - 15:30	**Kaffeepause 1**
15:30 - 17:30 **Seminarraum 30**	**WS 1b: Data processing in mass spectrometry imaging** Chair der Sitzung: **Andreas Römpp** Chair der Sitzung: **Bernhard Spengler** Andreas Römpp and Bernhard Spengler
15:30 - 17:30 **Seminarraum 26**	**WS 2b: Workshop "Core Facilities"** Chair der Sitzung: **Christof Lenz** Chair der Sitzung: **Sabine Metzger** Chair der Sitzung: **Axel Imhof** Christof Lenz, Universitäsmedizin Göttingen; Axel Imhof, Ludwig-Maximilians-Universität München
15:30 - 17:30 **Hörsaal 4**	**WS 3b: Lipidomics: A Workshop about Lipid Function and Analysis** Chair der Sitzung: **Robert Ahrends** Chair der Sitzung: **Dominik Schwudke** Chair der Sitzung: **Cristina Coman** Chair der Sitzung: **Andrej Shevchenko** Dominik Kopcynski,
15:30 - 17:30 **Seminarraum 31**	**WS 4b: Wissenschaftliches Publizieren** Chair der Sitzung: **Jürgen Gross** Chair der Sitzung: **Jürgen Grotemeyer**
15:30 - 17:30 **Hörsaal 2**	**WS 5b: Grundlagen der Massenspektrometrie** Chair der Sitzung: **Dietmar Kuck** Chair der Sitzung: **Matthias Letzel** Chair der Sitzung: **Mathias Schäfer**
18:00 - 18:30 **Hörsaal 3**	**Tagungseröffnung** Prof.Dr. A.Sinz, DGMS Vorsitzende, Prof.Dr. N.Oppelt, Dekanin, MNF, CAU Kiel, Prof.Dr. J.Grotemeyer, CAU Kiel
18:30 - 19:30 **Hörsaal 3**	**WP: Wolfgang-Paul-Vortrag** Chair der Sitzung: **Andrea Sinz**
	18:30 - 19:30 **ID: 180 / WP: 1** **Wolfgang-Paul-Vortrag** *Stichworte:* Cellular, machines, integrative, methods **Integrative Methods for Elucidating the Structure & Function of Cellular Machines** **Brian T. Chait** The Rockefeller University, New York, USA; Brian.Chait@rockefeller.edu WP-1-180.pdf
19:30 - 22:00 **Eingangshalle**	**Welcome Reception** Wir danken der Firma ThermoFisher Scientific für die freundliche Unterstützung des catering.

50. Jahrestagung der Deutschen Gesellschaft für Massenspektrometrie

Datum: Montag, 06.03.2017

8:00 - 16:00 — **Mo_Tag: Tagungsbüro**

8:30 - 8:35 — **Hörsaal 3**

Mo_Ank: Informationen

8:35 - 9:20 — **Hörsaal 3**

Plenarvortrag 1: MS Imaging
Chair der Sitzung: **Bernhard Spengler**

ID: 171 / **Plenarvortrag 1: 1**
Plenarvortrag
Stichworte: Imaging mass spectrometry, translational research, MALDI, SIMS

Translational mass spectrometry: Molecular images and more.

Ron M.A. Heeren
Maastricht University, Niederlande; r.heeren@maastrichtuniversity.nl

9:25 - 10:25 — **Hörsaal 3**

MoV_1a: Lipide I
Chair der Sitzung: **Robert Ahrends**

9:25 - 9:45
ID: 92 / **MoV_1a: 1**
Vortrag
Themen: Lipide & Lipidomics
Stichworte: UPLC-MS/MS of phospholipid positional isomers, positional analysis of fatty acids, mixed diacylglycerophospholipids, structure analysis of glycerophospholipids, quantitative fragment ion analysis

Quantitative Positional Isomer Analysis of Mixed Diacyl-Glycerophospholipids (dGPLs) by Ultra Performance Liquid Chromatography-Electrospray-Tandem Mass Spectrometry (UPLC-ESI-MS/MS)

Katharina Wozny[1], Wolf-Dieter Lehmann[1,2], Britta Brügger[1]
[1]Biochemie-Zentrum Heidelberg, Deutschland; [2]DKFZ Heidelberg; katharina.wozny@bzh.uni-heidelberg.de

MoV_1a-1-92.pdf

9:45 - 10:05
ID: 53 / **MoV_1a: 2**
Vortrag
Themen: Lipide & Lipidomics
Stichworte: neuronal lipis, HCD, lipidomics, lipid fragmentation, lipid quantification

Fragmentation behavior of neuronal lipids by HCD-MS/MS

Tommy Hofmann, Carla Schmidt
Interdisciplinary research center HALOmem, Martin Luther University Halle-Wittenberg, Kurt-Moses-Straße-3, 06120 Halle (Saale).; Tommy.Hofmann@biochemtech.uni-halle.de

MoV_1a-2-53.pdf

10:05 - 10:25
ID: 61 / **MoV_1a: 3**
Vortrag
Themen: MS - Informatik / Bioinformatik, Lipide & Lipidomics
Stichworte: Lipidomics, Lipid oxidation, LC-MS, Database, Systems medicine

oxLipidomics data integration for systems medicine view on metabolic diseases

Zhixu Ni[1,2], Georgia Angelidou[1,2], Giulia Coliva[1,2], Marina Armeni[1,2], Mike Lange[1,2], Maria Fedorova[1,2]
[1]Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig; [2]Center for Biotechnology and Biomedicine, Universität Leipzig, Germany; maria.fedorova@bbz.uni-leipzig.de

9:25 - 10:25 — **Hörsaal 2**

MoV_2a: Bildgebende Massenspektrometrie
Chair der Sitzung: **Andreas Römpp**

9:25 - 9:45
ID: 4 / **MoV_2a: 1**
Vortrag

Themen: Bildgebende Massenspektrometrie / MS Imaging, Lipide & Lipidomics
Stichworte: High resolution AP-SMALDI imaging, nematodes, Caenorhabditis elegans, neuronal lipids, sensory neurons

Differentiating wild and mutant C. elegans using high-resolution atmospheric pressure matrix assisted laser desorption/ionization mass spectrometry imaging

Saleh mahmud Khalil[1], Dhaka ram Bhandari[1], Thomas Hannich[2], Bernhard Spengler[1]
[1]Justus Liebig University Giessen, Institute of Inorganic and Analytical Chemistry; [2]University of Geneva, Department of Biochemistry; Saleh.M.Khalil@anorg.Chemie.uni-giessen.de

MoV_2a-1-4.pdf

9:45 - 10:05
ID: 2 / MoV_2a: 2
Vortrag
Themen: Bildgebende Massenspektrometrie / MS Imaging, Klinische Diagnostik & Forensik
Stichworte: bioimaging, photosensitizer, brain tumor, MALDI-MS, LA-ICP-MS

Bioimaging of photosensitizers in human brain tumors after fluorescence-guided resection

Sabrina Kröger[1], Ann-Christin Niehoff[1], Astrid Jeibmann[2], Walter Stummer[3], Uwe Karst[1]
[1]University of Münster, Institute of Inorganic and Analytical Chemistry, Münster, Germany; [2]University Hospital of Münster, Institute of Neuropathology, Münster, Germany; [3]University Hospital of Münster, Department of Neurosurgery, Münster, Germany; sabrina.kroeger@uni-muenster.de

MoV_2a-2-2.pdf

10:05 - 10:25
ID: 130 / MoV_2a: 3
Vortrag
Themen: Bildgebende Massenspektrometrie / MS Imaging, Element- & Speziationsanalytik
Stichworte: LA-ICP-MS, MALDI-MS, Imaging, Nanoparticles

Imaging of Cerium Oxide Nanoparticles and Phospholipids in Rat Lung Tissue by Means of LA-ICP-MS and MALDI-MS

Dörthe Dietrich[1], Antje Vennemann[2], Martin Wiemann[2], Michael Sperling[1,3], Uwe Karst[1]
[1]Westfälische Wilhelms-Universität Münster; [2]IBE R&D gGmbH; [3]European Virtual Institute for Speciation Analysis; doerthe.dietrich@uni-muenster.de

MoV_2a-3-130.pdf

9:25 - 10:25
Hörsaal 1

MoV_3a: Gasphasenreaktionen & Fragmentierungen I

Chair der Sitzung: **Dietmar Kuck**

9:25 - 9:45
ID: 13 / MoV_3a: 1
Vortrag
Themen: Gasphasenreaktionen & Fragmentierungen, Organische Massenspektrometrie
Stichworte: Hochauflösende Massenspektrometrie, Fragmentierungsreaktionen, Photodissoziation, DFT, RRKM

Energetische und kinetische Betrachtung der Fragmentierung von Azofarbstoffen mit Diethylamino Gruppe

Martin Clemen, Jürgen Grotemeyer
Christian-Albrechts-Universität zu Kiel, Institut für Physikalische Chemie, Max-Eyth-Str. 1, 24118 Kiel, Deutschland; clemen@phc.uni-kiel.de

MoV_3a-1-13.pdf

9:45 - 10:05
ID: 112 / MoV_3a: 2
Vortrag
Themen: Gasphasenreaktionen & Fragmentierungen, Organische Massenspektrometrie
Stichworte: Click Reaction, CuAAC, Gas-phase, Reaction Mechanism, Ion Chemistry

COPPER-CATALYSED CLICK REACTION PERFORMED IN THE GAS PHASE: A COMBINED MASS SPECTROMETRIC AND DFT MECHANISTIC STUDY

Claudio Iacobucci[1,2], Alexandre Lebon[1], Francesco De Angelis[3], Antony Memboeuf[1]
[1]UMR CNRS 6521, Université de Bretagne Occidentale, 6 Av.Le Gorgeu, 29200 Brest, France; [2]Institute of Pharmacy, Martin-Luther University Halle-Wittenberg, Halle/Saale, Germany, Deutschland; [3]Dipart. di Sci. Fisiche e Chimiche, Università degli Studi dell'Aquila, Via Vetoio, Coppito, 67100 L'Aquila, Italy; iacobucci.claudio@gmail.com

MoV_3a-2-112.pdf

10:05 - 10:25
ID: 150 / MoV_3a: 3

Vortrag
Themen: Gasphasenreaktionen & Fragmentierungen, Organische Massenspektrometrie
Stichworte: Electrospray ionization, FT-ICR mass spectrometry, benzyl halides, selective analysis, crude oil.

Electrospray Fourier Transform ion cyclotron resolution mass spectrometry: reactivity of polyaromantic heterocycles in heavy crude oils towards benzyl halides.

Xuxiao Wang, Wolfgang Schrader
Max-Planck-Institut für Kohlenforschung, Deutschland; wxuxiao@mpi-muelheim.mpg.de

MoV_3a-3-150.pdf

9:25 - 10:25
Hörsaal 4

MoV_4a: MS Analytik

Chair der Sitzung: **Hartmut Schlüter**

9:25 - 9:45
ID: 231 / MoV_4a: 1
Vortrag
Themen: Bildgebende Massenspektrometrie / MS Imaging, Element- & Speziationsanalytik
Stichworte: Triple quadrupole ICP-MS, Laser ablation, Wilson´s disease, Sulphur

Elemental Bioimaging by LA-ICP-QQQ-MS for the Investigation of Wilson´s Disease

Oliver Hachmöller[1], Peter Planitz[2], Michael Sperling[1,3], Uwe Karst[1]
[1]Institute of Inorganic and Analytical Chemistry, University of Münster, Münster, Germany; [2]Agilent Technologies, Waldbronn, Germany; [3]European Virtual Institute for Speciation Analysis (EVISA), Münster, Germany; hachmoeller@uni-muenster.de

MoV_4a-1-231.pdf

9:45 - 10:05
ID: 107 / MoV_4a: 2
Vortrag
Themen: Element- & Speziationsanalytik
Stichworte: Electrochemistry, Platinum cytostatics, LC-MS, Isotope Dilution

Electrochemical conversion of Pt(IV) prodrugs to Pt(II) cytostatics investigated by means of liquid chromatography and mass spectrometry

Lisa Frensemeier[1], Gunda Koellensperger[2], Bernhard K. Keppler[2], Christian R. Kowol[2], Uwe Karst[1]
[1]Universität Münster, Deutschland; [2]Universität Wien, Österreich; lisa.frensemeier@uni-muenster.de

MoV_4a-2-107.pdf

10:05 - 10:25
ID: 44 / MoV_4a: 3
Vortrag
Themen: Proteine & Proteomics, Lebensmittelanalytik
Stichworte: Oxidation, Protein carbonylation, Aldehyde reactive probe, Milk proteomics

Protein carbonylation in raw milk and differently processed milk products

Sanja Milkovska-Stamenova[1,2], Ruzanna Mnatsakanyan[1,2], Ralf Hoffmann[1,2]
[1]Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig; [2]Center for Biotechnology and Biomedicine, Universität Leipzig; sanja.milkovska@uni-leipzig.de

10:25 - 10:50 **Kaffeepause 2**

10:50 - 12:10
Hörsaal 3

MoV_1b: Lipide I

Chair der Sitzung: **Robert Ahrends**

10:50 - 11:10
ID: 11 / MoV_1b: 1
Vortrag
Themen: Lipide & Lipidomics
Stichworte: Lipidomics, Paternó-Büchi reaction, Charge switching, Double bond position

Charge Switching of Phospholipids using Paternó-Büchi Reactions

Patrick Esch, Bernhard Spengler, Sven Heiles
Institute of Inorganic and Analytical Chemistry, Justus-Liebig-University, Giessen, Germany; Patrick.Esch@anorg.chemie.uni-giessen.de

MoV_1b-1-11.pdf

11:10 - 11:30
ID: 163 / MoV_1b: 2

Vortrag
Themen: Lipide & Lipidomics
Stichworte: Lipid mediators, Spectra comparison score, HR-MS, quality control

Software platform to improve the quality control of Lipid mediator quantification

Adam Wutkowski[1], Navratan Bagwan[2], Matthias Krajewski[1], Bhesh Raj Paudyal[3], Ulrich E. Schaible[3], Mathias Schäfer[4], Dominik Schwudke[1]
[1]Division of Bioanalytical Chemistry, Research Center Borstel, Parkallee 10, Borstel, Germany; [2]Centro Nacional de investigaciones Cardiovasculares Carlos III (CNIC), Melchor Fernandez Almagro 3, 28029 Madrid, Spain; [3]Department of Cellular Microbiology, Research Center Borstel, Parkallee 22, Borstel, Germany; [4]Institute of Organic Chemistry, University of Cologne, Greinstraße 4, 50939 Köln, Germany; awutkowski@fz-borstel.de

MoV_1b-2-163.pdf

11:30 - 11:50
ID: 206 / MoV_1b: 3
Vortrag
Themen: Lipide & Lipidomics
Stichworte: lipidomics, colorectal cancer

Lipidomics reveals lipid networks correlated with the progression of human colorectal cancer

Yuting Wang[1,2], Kai Schuhmann[2], Sara Ciucci[3,4], Carlo V. Cannistraci[3], Mario Brosch[5], Andrej Shevchenko[2], Sebastian Zeissig[1,5]
[1]Center for Regenerative Therapies, Technical University Dresden, Dresden, Germany; [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany; [3]Biomedical Cybernetics Group, Biotechnology Center, Technical University Dresden, Dresden, Germany; [4]Lipotype GmbH, Dresden, Germany; [5]Department of Medicine I, University Medical Center Dresden, Technical University Dresden, Dresden, Germany; yuting.wang@crt-dresden.de

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11:50 - 12:10
ID: 142 / MoV_1b: 4
Vortrag
Themen: Lipide & Lipidomics
Stichworte: Lipidomics, Nano-LC

Development of a nanoLC-MS method for global lipidomics

Niklas Danne-Rasche, Robert Ahrends
Leibniz Institut für Analytische Wissenschaften ISAS e.V.; niklas.dannerasche@isas.de

MoV_1b-4-142.pdf

10:50 - 12:10
Hörsaal 2

MoV_2b: Bildgebende Massenspektrometrie

Chair der Sitzung: **Bernhard Spengler**

10:50 - 11:10
ID: 7 / MoV_2b: 1
Vortrag
Themen: Bildgebende Massenspektrometrie / MS Imaging, Instrumentelle Entwicklungen
Stichworte: Instrumentation, MALDI, Imaging

Implementation of a High Repetition-Rate Laser System in an AP-SMALDI MSI System for Enhanced Measurement Speed

Mario Kompauer, Max A. Mueller, Bernhard Spengler
Justus Liebig University Giessen, Germany; mario.kompauer@anorg.chemie.uni-giessen.de

MoV_2b-1-7.pdf

11:10 - 11:30
ID: 31 / MoV_2b: 2
Vortrag
Themen: Bildgebende Massenspektrometrie / MS Imaging
Stichworte: DESI, clinical research, molecular pathology

Getting DESI Imaging up to speed for clinical applications

Emrys Jones, Philippa J. Hart, Mark Towers, Sebastian Gottfried, Emmanuelle Claude
Waters Corporation, United Kingdom; sebastian_gottfried@waters.com

MoV_2b-2-31.pdf

11:30 - 11:50
ID: 129 / MoV_2b: 3
Vortrag
Themen: Bildgebende Massenspektrometrie / MS Imaging, Umweltanalytik
Stichworte: Imaging, LA-ICP-MS, metamorphosis, ecosystem

Investigating the zinc distribution in the mayfly N. triangulifer using elemental bioimaging by LA-ICP-MS

Barbara Crone[1], Janet Miller[2], Johanna Kraus[2], Travis Schmidt[2], David Walters[2], Uwe Karst[1]
[1]Institut für Anorganische und Analytische Chemie, Universität Münster, Deutschland; [2]Fort Collins Science Center, US Geological Survey, Fort Collins, USA; barbaracrone@uni-muenster.de

MoV_2b-3-129.pdf

11:50 - 12:10
ID: 104 / MoV_2b: 4
Vortrag
Themen: Bildgebende Massenspektrometrie / MS Imaging
Stichworte: MS imaging, imzML, data processing, data standard, multimodal imaging

imzML - Current status and future perspectives of the open standard for mass spectrometry imaging data

Nicolas Desbenoit, Amol Fatangare, Andreas Römpp
Chair of Bioanalytical Sciences and Food Analysis, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth, Germany; andreas.roempp@uni-bayreuth.de

10:50 - 12:10
Hörsaal 1

MoV_3b: Grundlagen und Instrumentelle Entwicklungen I

Chair der Sitzung: **Mathias Schäfer**

10:50 - 11:10
ID: 74 / MoV_3b: 1
Vortrag
Themen: Grundlagen der Massenspektrometrie, Ionisationsmethoden
Stichworte: cryospray ionization, electrospray ionization, internal energy, thermometer ions

Internal energy of ions produced by electrospray and cryospray ionization

Friedrich Kreyenschmidt, Thomas Auth, Konrad Koszinowski
Georg-August-Universität Göttingen, Deutschland; konrad.koszinowski@chemie.uni-goettingen.de

MoV_3b-1-74.pdf

11:10 - 11:30
ID: 57 / MoV_3b: 2
Vortrag
Themen: Bildgebende Massenspektrometrie / MS Imaging, Instrumentelle Entwicklungen
Stichworte: LAESI, Mass Spectrometry Imaging, Profilometry

Mapping metabolites from rough terrain: laser ablation electrospray ionization on non-flat samples

Benjamin Bartels[1], Purva Kulkarni[1,2], Sebastian Böcker[2], Norbert Danz[3], Hans Peter Saluz[4], Aleš Svatoš[1]
[1]Research Group Mass spectrometry/Proteomics, Max Planck Institute for Chemical Ecology; [2]Chair for Bioinformatics, Friedrich Schiller University Jena; [3]Fraunhofer Institute for Applied Optics and Precision Engineering IOF; [4]Department Cell and Molecular Biology, Leibniz Institute for Natural Product Research and Infection Biology; bbartels@ice.mpg.de

MoV_3b-2-57.pdf

11:30 - 11:50
ID: 27 / MoV_3b: 3
Vortrag
Themen: Grundlagen der Massenspektrometrie, Ionisationsmethoden
Stichworte: MALDI, desorption, ablation, spot size dependence, velocity distribution

New insights into the MALDI mechanisms: Postionization and photoacoustic experiments reveal laser spot size-dependent transitions between desorption and ablation regimes

Marcel Wiegelmann[1], Klaus Dreisewerd[1,2], Jens Soltwisch[1,2]
[1]Institute for Hygiene, Biomedical Mass Spectrometry, University of Münster, Germany; [2]Interdisciplinary Center for Clinical Research (IZKF), University of Münster, Germany; marcel.wiegelmann@ukmuenster.de

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11:50 - 12:10
ID: 71 / MoV_3b: 4
Vortrag
Themen: Grundlagen der Massenspektrometrie, Lipide & Lipidomics
Stichworte: MALDI-TOF MS; Adipose Tissue; Phospholipids; Ion Suppression; CsCl.

Selective triacylglycerol suppression in complex lipid mixtures by CsCl addition

Yulia Popkova, Jürgen Schiller

Leipzig University, Faculty of Medicine, Institute for Medical Physics and Biophysics, Germany; yulia.popkova@medizin.uni-leipzig.de

MoV_3b-4-71.pdf

10:50 - 12:10
Hörsaal 4

MoV_4b: Klinische Diagnostik & Forensic

Chair der Sitzung: **Hartmut Schlüter**

10:50 - 11:10
ID: 176 / MoV_4b: 1
Vortrag
Themen: Klinische Diagnostik & Forensik, Metaboliten & Metabolomics
Stichworte: Backdoorpathway Androgene

Entwicklung einer LC-MS/MS Methode zur Bestimmung der Backdoorpathway Hormone Androsterone und Androstandiol und der Androgene Androstendion, Testosteron und Dihydrotestosteron

Alexandra Kulle, Helena Wulf, Paul-Martin Holterhus
Universitätsklinikum Schleswig-Holstein, Deutschland; Alexandra.kulle@uksh.de

MoV_4b-1-176.pdf

11:10 - 11:30
ID: 178 / MoV_4b: 2
Vortrag
Themen: Klinische Diagnostik & Forensik
Stichworte: Vitamin D, Epimers, Dried Blood Spots, Serum

Vitamin D3 epimers: analytical nuisance or clinical opportunity?

Dietrich Volmer[1], Miriam Müller[1], Caroline Stokes[2]
[1]Universität des Saarlandes, Saarbrücken, Deutschland; [2]Universitätsklinikum des Saarlandes, Homburg, Deutschland; dietrich.volmer@mx.uni-saarland.de

MoV_4b-2-178.pdf

11:30 - 11:50
ID: 138 / MoV_4b: 3
Vortrag
Themen: Klinische Diagnostik & Forensik, Proteine & Proteomics
Stichworte: ERLIC, Phosphoproteomics, Parellel reaction monitoring, Cancer

Excellent sensitivity through excellent recovery – ERLIC for absolute quantification of low abundant protein phosphorylation events in cancer patient tissue

Stefan Loroch[1], Giusy DiConza[2], Massimiliano Mazzone[2], René Zahedi[1], Albert Sickmann[1,3,4]
[1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund, Germany; [2]Laboratory of Molecular Oncology and Angiogenesis, Vesalius Research Center, Leuven, Belgium; [3]Department of Chemistry, College of Physical Sciences, University of Aberdeen, United Kingdom; [4]Medizinisches Proteom Center, Ruhr Universität Bochum, Germany; stefan.loroch@isas.de

MoV_4b-3-138.pdf

11:50 - 12:10
ID: 242 / MoV_4b: 4
Vortrag
Themen: Bildgebende Massenspektrometrie / MS Imaging, Klinische Diagnostik & Forensik
Stichworte: MALDI-MS imaging, ion-mobility separation, amyloidosis, formalin-fixiert/paraffin-embedded

Identification and classification of amyloidosis by matrix-assisted laser desorption/ionization mass spectrometry imaging

Martin Winter[1], Andreas Tholey[2], Christoph Röcken[1]
[1]Institute of Pathology, Christian-Albrechts-Universität, Kiel, Germany; [2]Systematic Proteome Research & Bioanalytics, Institute of Experimental Medicine, Christian-Albrechts-Universität, Kiel, Germany; martin.winter@uksh.de

MoV_4b-4-242.pdf

12:15 - 14:00
Seminarraum 30

Lunch 1: Lunchseminar Thermo

Spezielle Registrierung bei der Firma

12:15 - 14:00
Hörsaal 2

Lunch 2: Lunchseminar Waters

Spezielle Registrierung bei der Firma

12:15 - 14:00
Hörsaal 4

Lunch 3: Lunchseminar Shimadzu

Spezielle Registrierung bei der Firma

14:00 - 14:45

Hörsaal 3	**Plenarvortrag 2: "Nucleic acids biophysics"** Chair der Sitzung: **Michael Linscheid**

ID: 249 / Plenarvortrag 2: 1
Plenarvortrag

Nucleic acids biophysics: insight from (and into) mass spectrometry

Valérie Gabelica
Inserm, CNRS, Université de Bordeaux, Laboratoire "Acides Nucléiques, Régulations Naturellee et Artificielle" (ARNA, U1212, UMR5320), IECB, Pessac, France; valerie.gabelica@inserm.fr

14:45 - 15:30 **Hörsaal 3**	**Mo_Pr: Preisverleihung Wolfgang-Paul-Studienpreis** Chair der Sitzung: **Mathias Schäfer** Preisträger: Frau Dr. Niehoff Herr Dr. Kwiatkowski

ID: 252 / Mo_Pr: 1
Vortrag
Themen: Sonstiges
Stichworte: MALDI, Ablation

Mass Spectrometric Characterization of Proteins from condensates of the Picosecond Infrared Laser Ablation

Marcel Kwiatkowski[1,2]
[1]University Medical Center Groningen, Department of Pulmonary Diseases and Tuberculosis, Groningen, The Netherlands.; [2]University of Groningen, Department of Analytical Biochemistry, The Netherlands.; m.kwiatkowski@rug.nl

15:30 - 16:00	**Kaffeepause 3**
16:00 - 18:00 **Hörsaal 3**	**MoN_1a: Proteine & Proteomics I** Chair der Sitzung: **Wolf-Dieter Lehmann**

16:00 - 16:20
ID: 137 / MoN_1a: 1
Vortrag
Themen: Proteine & Proteomics
Stichworte: Cross-linking, oligomerisation, protein interactions, protein-lipid interactions

Ligand induced oligomerisation of proteins – insights from mass spectrometry

Carla Schmidt
Interdisciplinary research center HALOmem, Martin Luther University University Halle-Wittenberg; carla.schmidt@biochemtech.uni-halle.de

MoN_1a-1-137.pdf

16:20 - 16:40
ID: 243 / MoN_1a: 2
Vortrag
Themen: Klinische Diagnostik & Forensik, Proteine & Proteomics
Stichworte: Proteomics, phosphoproteomics, quantitative mass spectrometry, biomarker

Temporal quantitative phosphoproteomics of ADP stimulation reveals novel central nodes in platelet activation and inhibition

Florian Beck[1], Jörg Geiger[2], Stepan Gambaryan[3], Fiorella A. Solari[1], Margherita Dell'Aica[1], Stefan Loroch[1], Nadine J. Mattheij[4], Igor Mindukshev[3], Oliver Pötz[5], Kerstin Jurk[6], Julia M. Burkhart[1], Christian Fufezan[7], Johan W. M. Heemskerk[4], Ulrich Walter[6], Rene P. Zahedi[1], Albert Sickmann[1]
[1]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Deutschland; [2]Interdisciplinary Bank of Biomaterials and Data, Würzburg, Germany;; [3]Sechenov Institute of Evolutionary Physiology and Biochemistry, Russian Academy of Sciences, Saint Petersburg, Russia;; [4]Department of Biochemistry, Cardiovascular Research Institute Maastricht, Maastricht University, The Netherlands;; [5]Natural and Medical Sciences Institute at the University of Tübingen, Tübingen, Germany;; [6]Center for Thrombosis and Hemostasis, Universitätsklinikum der Johannes Gutenberg-Universität Mainz, Mainz, Germany;; [7]Institute for Biology and Biotechnology of Plants, University Münster, Münster, Germany;; sickmann@isas.de

MoN_1a-2-243.pdf

16:40 - 17:00
ID: 81 / MoN_1a: 3
Vortrag
Themen: Proteine & Proteomics
Stichworte: Calmodulin, Munc13, Cross-Linking, photo-methionine

Cross-Linking and Mass Spectrometry Shed New Light on the bMunc13-2/Calmodulin Interaction

Christine Piotrowski[1], Olaf Jahn[2], Christian Ihling[1], Jens Meiler[3], Andrea Sinz[1]
[1]Martin-Luther-Universität Halle-Wittenberg, Deutschland; [2]Max-Planck-Institut für Experimentelle Medizin, Göttingen, Deutschland; [3]Vanderbilt University, Nashville, Tennessee, USA;
christine.piotrowski@pharmazie.uni-halle.de

MoN_1a-3-81.pdf

17:00 - 17:20
ID: 225 / MoN_1a: 4
Vortrag
Themen: Proteine & Proteomics
Stichworte: Capture compounds (CC), ICP-MS

Metal labelling of tri-functional Capture Compounds (CCs) to detect protein targets of small molecules

Oleksandra Kuzmich[1], Thomas Lenz[2], Simon Michaelis[2], Matthias Hakelberg[2], Uschi Gruber[2], Mathias Dreger[2], Michael Linscheid[1]
[1]Humboldt Universität zu Berlin, Deutschland; [2]caprotec bioanalytics GmbH;
aleksandrakuzmich@gmail.com

MoN_1a-4-225.pdf

17:20 - 17:40
ID: 63 / MoN_1a: 5
Vortrag
Themen: Proteine & Proteomics
Stichworte: Peptide pyrophosphorylation, neutral-loss-trigger, EThcD

Neutral loss-triggered EThcD mass spectrometry identifies protein pyrophosphorylation in vivo

Martin Penkert[1,2], Lisa M. Yates[3], Michael Schümann[1], Dorothea Fiedler[1,2,3], Eberhard Krause[1]
[1]Leibniz-Institut für molekulare Pharmakologie (FMP), Deutschland; [2]Humboldt-Universität zu Berlin; [3]Princeton University; penkert@fmp-berlin.de

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17:40 - 18:00
ID: 134 / MoN_1a: 6
Vortrag
Themen: Proteine & Proteomics
Stichworte: Proteostasis, HSP90, primary cells, PROTAC

Analysis of drug-induced effects on proteostasis in cell lines and non-dividing primary cells by quantitative mass spectrometry

Nico Zinn[1], Mikhail M. Savitski[1,2], Maria Faelth-Savitski[1], Daniel Poeckel[1], Johanna Vappiani[1], Katrin Müller[1], Anne Wagner[1], Holger Franken[1], Stephan Gade[1], Marcel Mülbaier[1], Giovanna Bergamini[1], Marcus Bantscheff[1]
[1]Cellzome GmbH, Heidelberg; [2]EMBL, Heidelberg; nico.x.zinn@gsk.com

MoN_1a-6-134.pdf

16:00 - 18:00
Hörsaal 2

MoN_2a: Analytische Anwendungen I

Chair der Sitzung: **Michael Karas**

16:00 - 16:20
ID: 105 / MoN_2a: 1
Vortrag
Themen: Klinische Diagnostik & Forensik, Organische Massenspektrometrie
Stichworte: fuel additives, brand recognition, LC-ESI-MS, structure identification, database

Development and implementation of new analytical methods and databases for the detection of additives in fuels and fire debris.

Lisa Scharrenbroch[1,2], Dieter Kirsch[1], Sandra Kasuch[1], Paula Eckelmann[1,3], Frank Schäfer[1], Niamh NicDaeid[2], René de Bruyn[4], Xiaoma Xu[4], Michiel Grutters[4], Jeanet Hendrikse[4]
[1]Federal Criminal Police Office, Forensic Institute, 65193 Wiesbaden, Germany; [2]University of Dundee, CAHID, School of Science and Engineering, Dundee, DD15EH, Scotland; [3]Justus-Liebig-University Giessen, Institute of Food Chemistry and Food Biotechnology, 35392 Giessen, Germany; [4]Netherlands Forensic Institute, Forensic Chemistry – Chemical Identification Analysis, 2497 GB The Hague, Netherlands; lisascha92@freenet.de

MoN_2a-1-105.pdf

16:20 - 16:40
ID: 76 / MoN_2a: 2
Vortrag

Themen: Umweltanalytik, Sonstiges
Stichworte: Lignin characterization, Ambient ionization, High resolution mass spectrometry, Mass defect filtering, Renewable energy

Rapid fingerprinting of lignin renewable energy sources by ambient ionization high-resolution mass spectrometry and simplified data mining

Elizabeth Crawford[1], Stefanie Gerbig[2], Bernhard Spengler[2], Dietrich Volmer[1]
[1]Saarland University, Saarbrücken, Deutschland; [2]Justus Liebig University, Gießen, Deutschland; elizabeth.crawford@uni-saarland.de

MoN_2a-2-76.pdf

16:40 - 17:00
ID: 16 / MoN_2a: 3
Vortrag
Themen: Bildgebende Massenspektrometrie / MS Imaging, Metaboliten & Metabolomics
Stichworte: Mass spectrometry imaging, Atmospheric pressure Matrix Assisted Laser Desorption/Ionization, Schistosomiasis

AP-SMALDI MSI of metabolites and lipids in Schistosoma mansoni parasites

Patrik Kadesch[1], Thomas Quack[2], Stefanie Gerbig[1], Christoph Grevelding[2], Bernhard Spengler[1]
[1]Justus-Liebig-Universität Gießen, Institut für Anorganische und Analytische Chemie; [2]Justus-Liebig-Universität Gießen, Institut für Parasitologie; patrik.kadesch@anorg.chemie.uni-giessen.de

MoN_2a-3-16.pdf

17:00 - 17:20
ID: 23 / MoN_2a: 4
Vortrag
Themen: Umweltanalytik
Stichworte: Water-extractable organic matter, laser-desorption/ionization time-of-flight mass spectrometry, nuclear magnetic resonance spectroscopy, nonmetric multidimensional scaling, fire disturbance

Effect of ecosystem type and fire on chemistry of WEOM as measured by LDI-TOF-MS and NMR

Anna C. Crecelius, Jürgen Vitz, Kerstin Näthe, Stefanie Meyer, Beate Michalzik, Ulrich S. Schubert
Friedrich Schiller University Jena, Deutschland; anna.crecelius@uni-jena.de

MoN_2a-4-23.pdf

17:20 - 17:40
ID: 229 / MoN_2a: 5
Vortrag
Themen: Instrumentelle Entwicklungen, Umweltanalytik
Stichworte: high resolution mass spectrometry, evolved gas analysis, atmospheric pressure ionisation, petroleomics, combustion aerosol

Evolved gas analysis ultra high resolution mass spectrometry - Insights into heavy petroleum fractions and combustion aerosol

Christopher Paul Rüger[1], Anika Neumann[1], Martin Sklorz[1], Theo Schwemer[1,2], Ralf Zimmermann[1,2,3]
[1]Joint Mass Spectrometry Centre / Chair of Analytical Chemistry, University of Rostock, 18059 Rostock, Germany; [2]HICE - Helmholtz Virtual of Complex Molecular Systems in Environmental Health – Aerosols and Health, www.hice-vi.eu; [3]Cooperation Group Comprehensive Molecular Analytics, Helmholtz Zentrum München, 85764 Neuherberg, Germany; christopher.rueger@uni-rostock.de

MoN_2a-5-229.pdf

ID: 9 / MoN_2a: 6
Vortrag
Themen: Proteine & Proteomics
Stichworte: LC-MS/MS, development, database, SILAC, label-free quantitation

Proteomic resources for organismal development

Falk Butter
Institute of Molecular Biology, Deutschland; f.butter@imb.de

16:00 - 18:00
Hörsaal 1

MoN_3a: Ionisationsmethoden

Chair der Sitzung: **Matthias Letzel**

16:00 - 16:20
ID: 54 / MoN_3a: 1

Vortrag
Themen: Instrumentelle Entwicklungen, Ionisationsmethoden
Stichworte: photoionisation, crude oil, thermal analysis, evolved gas analysis

Direct resonance-enhanced multi-photon ionisation (REMPI) of complex liquid samples under vacuum conditions

Hendryk Czech[1], Claudia Kruth[1], Martin Sklorz[1], Johannes Passig[1], Ralf Zimmermann[1,2]
[1]Universität Rostock, Deutschland; [2]Helmholtz-Zentrum München, Deutschland; hendryk.czech@uni-rostock.de

MoN_3a-1-54.pdf

16:20 - 16:40
ID: 8 / MoN_3a: 2
Vortrag
Themen: Instrumentelle Entwicklungen, Ionisationsmethoden
Stichworte: Ionisation, API, electrospray, efficiency, aerodynamics

The Aerodynamics of Impactor Spray Ionisation Sources

Steve Bajic
Waters Corporation, United Kingdom; steve_bajic@waters.com

MoN_3a-2-8.pdf

16:40 - 17:00
ID: 18 / MoN_3a: 3
Vortrag
Themen: Ionisationsmethoden
Stichworte: Reactive low temperature plasma, ambient mass spectrometry, neurosteroid analysis

Reactive low temperature plasma (LTP) mass spectrometry of neurosteroids

Xuelu Ding, Sven Heiles, Bernhard Spengler
Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen; xuelu.ding@anorg.chemie.uni-giessen.de

MoN_3a-3-18.pdf

17:00 - 17:20
ID: 75 / MoN_3a: 4
Vortrag
Themen: Instrumentelle Entwicklungen, Ionisationsmethoden
Stichworte: DBDI-MS, Ambient-MS, TATP, Peroxid

Analyse des Peroxid-basierten Sprengstoffs TATP und strukturell verwandter Verbindungen mittels dielektrisch behinderter Entladungsionisations-Massenspektrometrie (DBDI-MS)

Sebastian Hagenhoff[1], Joachim Franzke[2], Heiko Hayen[1]
[1]Westfälische Wilhelms-Universität Münster; [2]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V.; hagenhoff@uni-muenster.de

MoN_3a-4-75.pdf

17:20 - 17:40
ID: 68 / MoN_3a: 5
Vortrag
Themen: Ionisationsmethoden
Stichworte: ambient mass spectrometry, aromatic amines, ionization efficiency, low temperature plasma

Impact factors on signal response with low temperature plasma ionization for mass spectrometry

Andreas Kiontke[1], Aigerim Galyamova[2], Claudia Birkemeyer[1]
[1]Universität Leipzig, Deutschland; [2]Pennsylvania State University, USA; andreas.kiontke@uni-leipzig.de

MoN_3a-5-68.pdf

17:40 - 18:00
ID: 120 / MoN_3a: 6
Vortrag
Themen: Instrumentelle Entwicklungen, Ionisationsmethoden
Stichworte: soft electron ionisation, GC-TOF MS, multiplexing

FAST MULTIPLEXING OF IONISATION ENERGY FOR PERFORMANCE IMPROVEMENTS IN GC-TOF MS

Gerhard Horner[1], **Jörg Köhler**[2], **Ruslan Dedishov**[2], **Thomas Zanni**[2], **Stefan Koschinski**[2], **Laura McGregor**[3], **Nick Bukowski**[3]
[1]Five Technologies GmbH, Frauenstrasse 22, 80469 Munich, Germany; [2]Markes International GmbH, Schleussnerstrasse 42, Frankfurt, Germany; [3]Markes International, Gwaun Elai Medi-Science Campus, Llantrisant, RCT, Wales, United Kingdom; g.horner@fivetechno.de

18:00 - 20:30
Eingangshalle

Poster: Poster Session Montag Abend

Autoren der Poster mit ungrader Posternummer sind anwesend.

ID: 244 / Poster: 1
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Grundlagen der Massenspektrometrie
Stichworte: McLafferty reaction, Substituent effects, Distonic ions, Hydrogen transfer, Proton affinity

2-Benzylindane radical cations in the gas phase (I): Substituent effects on a stereoselective McLafferty reaction and related hydrogen transfer processes

Hans-Friedrich Grützmacher, Dietmar Kuck
Department of Chemistry, Bielefeld University; dietmar.kuck@uni-bielefeld.de

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ID: 246 / Poster: 2
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Grundlagen der Massenspektrometrie
Stichworte: Hydrogen scrambling, McLafferty reaction, Substituent effects, Lifetime of ions, stereoselectivity

2-Benzylindane radical cations in the gas phase (II): Substituenteffects on regio- and stereoselective progressive hydrogen scramblingoccurring prior to unimolecular fragmentation

Dietmar Kuck, Hans-Friedrich Grützmacher
Department of Chemistry, Bielefeld University; dietmar.kuck@uni-bielefeld.de

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ID: 19 / Poster: 3
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Organische Massenspektrometrie
Stichworte: REMPI, Flugzeitmassenspektrometrie, Cluster

REMPI-Spektroskopie von nicht-kovalenten Anisol-Clustern

Thorben Reinert, Jürgen Grotemeyer
Christian-Albrechts-Universität zu Kiel, Deutschland; reinert@phc.uni-kiel.de

Poster-3-19.pdf

ID: 22 / Poster: 4
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Instrumentelle Entwicklungen
Stichworte: mass spectrometry, fullerenes, instrumentation, single particle analysis

Resolution enhancement by delayed ion extraction in a single-particle aerosol mass spectrometer

Christof Barth, Klaus Peter Hinz, Bernhard Spengler
Justus-Liebig Universität Giessen, Deutschland; christof.barth@chemie.uni-giessen.de

Poster-4-22.pdf

ID: 26 / Poster: 5
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Ionisationsmethoden
Stichworte: electrospray, phthalocyanine, crown ether, cluster, aggregate

Aggregation of a crown-ether decorated zinc-phthalocyanine by collision-induced desolvation providing insight into the electrospray mechanism

Ina Kellner[1], **Uwe Hahn**[2,3], **Maximilian Dürr**[1], **Tomás Torres**[2,4], **Ivana Ivanović-Burmacović**[1], **Thomas Drewello**[1]
[1]Friedrich-Alexander-University Erlangen-Nürnberg, Deutschland; [2]Universidad Autónoma de Madrid, Spain; [3]University of Strasbourg and CNRS, European School for Chemistry, Polymers and Materials (ECPM), France; [4]Instituto Madrileño de Estudios Avanzados (IMDEA)-Nanociencia, Spain; ina.kellner@fau.de

Poster-5-26.pdf

ID: 42 / Poster: 6
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Sonstiges

Stichworte: ESI Mass Spectrometry, Gas-Phase Reactivity, Reaction Intermediates, Kinetics, Reaction Mechanism

Direct Observation and Reactivity Studies of Organoferrates by Electrospray Ionization Mass Spectrometry

Tobias Parchomyk, Konrad Koszinowski
Georg-August-Universität Göttingen, Deutschland; tobias.parchomyk@chemie.uni-goettingen.de

Poster-6-42.pdf

ID: 33 / Poster: 7
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Proteine & Proteomics
Stichworte: Proteomics, Top-Down, Intact Protein, Electrospray Ionization, Collision-Induced Dissociation

Improving the sequence coverage in top-down MS/MS of proteins

Alexander Becker, Mohamed Mokhtar, Andreas Tholey
Christian-Albrechts-Universität zu Kiel, Deutschland; a.becker@iem.uni-kiel.de

Poster-7-33.pdf

ID: 95 / Poster: 8
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Organische Massenspektrometrie
Stichworte: Organometallic reagents – ESI mass spectrometry – gas phase reactivity – homogenous catalysis – cross-coupling

Constitution and gas phase reactivity of organocobaltates

Friedrich Kreyenschmidt, Konrad Koszinowski
Georg-August-Universität Göttingen, Institut für Organische und Biomolekulare Chemie; fkreyen@gwdg.de

Poster-8-95.pdf

ID: 5 / Poster: 9
Poster
Themen: Grundlagen der Massenspektrometrie, Instrumentelle Entwicklungen
Stichworte: Instrumentation, tandem mass spectrometry, UVPD, charge dependence, nESI

Implementation of Ultraviolet Photodissociation on a LTQ FT Ultra Mass Spectrometer and first Applications

Simon Becher, Mario Kompauer, Bernhard Spengler, Sven Heiles
Institut für Anorganische und Analytische Chemie; Justus-Liebig-Universität Gießen; Sven.Heiles@anorg.chemie.uni-giessen.de

Poster-9-5.pdf

ID: 169 / Poster: 10
Poster
Themen: Grundlagen der Massenspektrometrie, Ionisationsmethoden
Stichworte: MALDI plume, wavelength dependence, laser fluence, thermometer molecules, internal energies

The internal energy in a MALDI plume probed with thermometer molecules: Effects of laser excitation wavelength and laser fluence

Alexander Potthoff[1], Jens Soltwisch[1,2], Annika Koch[1], Klaus Dreisewerd[1,2]
[1]Institute for Hygiene, University of Münster, Robert-Koch-Str. 41, 48149 Münster, Germany; [2]Interdisciplinary Center for Clinical Research (IZKF), University of Münster, Domagkstr. 3, 48149 Münster, Germany; alexpotthoff@uni-muenster.de

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ID: 47 / Poster: 11
Poster
Themen: Grundlagen der Massenspektrometrie
Stichworte: MALDI-MS Imaging, MALDI matrix, Laser wavelength, Absorption profile, Ion yield

Colorful MALDI: Effect of the Laser Excitation Wavelength on the Analytical Sensitivity in Standard MALDI-MS and Imaging Experiments

Annika Koch[1], Jens Soltwisch[1], Klaus Dreisewerd[1,2]
[1]University of Münster, Institute of Hygiene, Biomedical Mass Spectrometry, Germany; [2]Interdisciplinary Center for Clinical Research (IZKF) Münster, Germany; annika.koch@uni-muenster.de

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ID: 14 / Poster: 12
Poster

Themen: Grundlagen der Massenspektrometrie, Ionisationsmethoden
Stichworte: Atmosphärenbedingungen, Cluster, LTP, Twin-Trap, Cassini-Falle

Untersuchung von Limonen-Clustern im LTP-Twin-Trap Massenspektrometer

Björn Raupers[1], Claus Köster[2], Jürgen Grotemeyer[1]
[1]Universität Kiel, Deutschland; [2]Bruker-Daltonik GmbH, Bremen; raupers@phc.uni-kiel.de

Poster-12-14.pdf

ID: 103 / Poster: 13
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Grundlagen der Massenspektrometrie
Stichworte: thermometer ions, dissociation energy, kinetic shift, SSACM

An improved approach for calculating dissociation rates of benzylpyridinium ions

Thomas Auth, Konrad Koszinowski
Institut für Organische und Biomolekuare Chemie, Georg-August-Universität Göttingen, Deutschland; thomas.auth@chemie.uni-goettingen.de

Poster-13-103.pdf

ID: 70 / Poster: 14
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Organische Massenspektrometrie
Stichworte: ESI-MS, gas-phase chemistry, palladium-catalyzed cross-coupling, catalyst activation

Stability and Unimolecular Reactivity of Organopalladate(II) Complexes

Marlene Kolter, Konrad Koszinowski
Georg-August-Universität Göttingen, Deutschland; marlene.kolter@chemie.uni-goettingen.de

Poster-14-70.pdf

ID: 48 / Poster: 15
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Organische Massenspektrometrie
Stichworte: coinage metals, ate-complexes, organometallic compounds, reactive intermediates

Coinage-Metal Ate Complexes – An ESI-MS Study

Sebastian Weske[1], Richard O'Hair[2], Konrad Koszinowski[1]
[1]Georg-August-University Göttingen, Germany; [2]University of Melbourne, Australia; sebastian.weske@chemie.uni-goettingen.de

Poster-15-48.pdf

ID: 123 / Poster: 16
Poster
Themen: Gasphasenreaktionen & Fragmentierungen
Stichworte: ETD, metallo-supramolecular-aggregates, one-electron reduction, self-assembly, gas phase reactivity

ETD experiments on self-assembled asymmetric supramolecular squares

Yvonne Lorenz, Marianne Engeser
Universität Bonn, Deutschland; ylorenz@uni-bonn.de

Poster-16-123.pdf

ID: 86 / Poster: 17
Poster
Themen: Gasphasenreaktionen & Fragmentierungen
Stichworte: Ag+ adducts, helicene, π-π stacking, Energy-dependent CID

Formation and structure elucidation of [M_2 and Ag]$^+$ ions with M = [6]helicene, [7]helicene and coronene

Vera Warmbrunn, Martin Minameyer, Thomas Drewello
Friedrich-Alexander-University Erlangen-Nürnberg, Germany; vera.warmbrunn@fau.de

Poster-17-86.pdf

ID: 88 / Poster: 18
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Grundlagen der Massenspektrometrie
Stichworte: Crystallization, fragmentation behavior, slow heating CID, resonant ion excitation, quadrupole ion trap

Formation and dissociation behavior of multiply charged salt-like cluster ions (sodium formate)

Thomas Neugebauer, Thomas Drewello

Friedrich-Alexander-University Erlangen-Nürnberg, Deutschland; thomas.neugebauer@fau.de

Poster-18-88.pdf

ID: 65 / Poster: 19
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Grundlagen der Massenspektrometrie
Stichworte: Photodissoziation, CID, FT-ICR, Laserfarbstoffe

Wellenlängenabhängige Photofragmentierung von fluoreszierenden Farbstoffen in einem FT-ICR Massenspektrometer

Elena Mitrofanov, Tassilo Muskat, Jürgen Grotemeyer
Christian-Albrechts-Universität, Deutschland; mitrofanov@phc.uni-kiel.de

Poster-19-65.pdf

ID: 39 / Poster: 20
Poster
Themen: Klinische Diagnostik & Forensik
Stichworte: New psychoactive substances; NPS; library; LC-MS/MS; QTrap;

Update of an MS/MS Library of NPS for QTRAP® instruments

Katharina Grafinger[1], Lars Ambach[1,2], Florian Franz[3], Verena Angerer[3], Wolgang Weinmann[1]
[1]Universtität Bern, Institut für Rechtsmedizin, Forensische Toxikologie und Chemie, Switzerland; [2]Universität Ghent, Department of Bioanalysis, Laboratory of Toxicology, Belgium; [3]Universitätsklinikum Freiburg, Institut für Rechtsmedizin, Forensische Toxikologie, Germany; katharina.grafinger@irm.unibe.ch

Poster-20-39.pdf

ID: 106 / Poster: 21
Poster
Themen: Klinische Diagnostik & Forensik
Stichworte: LC-MS, antibiotics, tuberculosis, therapeutic drug monitoring

LC-MS2 Method Development for Simultaneous Analysis of Antibiotics from Plasma of MDR-TB Patients

Hande Karaköse[1,3], Niklas Köhler[2,3], Christoph Lange[2,3,4], Patricia Sanchez-Carballo[2,3], Dominik Schwudke[1,3]
[1]Division of Bioanalytical Chemistry, Research Center Borstel, Germany; [2]Division of Clinical Infectious Diseases, Research Center Borstel, Borstel, Germany; [3]German Center for Infection Research, Clinical Tuberculosis Center, Borstel, Germany; [4]International Health/Infectious Diseases, University of Lübeck, Lübeck, Germany; hkarakoese@fz-borstel.de

Poster-21-106.pdf

ID: 200 / Poster: 22
Poster
Themen: Ionisationsmethoden, Native MS
Stichworte: Atmosphärendruck Ionisation, Papierbasierte Massenspektrometrie, Mikrofluidik, Instrumentelle Entwicklung

Modifikation von Papiersubstraten mit hydrophoben Barrieren zur Erhöhung der Empfindlichkeit und Reproduzierbarkeit in der papierbasierten Massenspektrometrie

Yves U. Hachenberger[1], Knut Rurack[2], Michael W. Linscheid[1], Jens Riedel[2]
[1]Humboldt-Universität zu Berlin; [2]Bundesanstalt für Materialforschung und -prüfung; Yves.Hachenberger@gmx.de

Poster-22-200.pdf

ID: 160 / Poster: 23
Poster
Themen: Ionisationsmethoden, Organische Massenspektrometrie
Stichworte: Pyrolysis bio-oil, Ionization techniques, Composition analysis

Characterization of Fast-Pyrolysis Bio-Oil

Yun Xu, Wolfgang Schrader
Max-Planck-Institut für Kohlenforschung, Deutschland; yxu@kofo.mpg.de

Poster-23-160.pdf

ID: 77 / Poster: 24
Poster
Themen: Ionisationsmethoden, Umweltanalytik
Stichworte: Nano Particle Analysis, Extractive Electrospray Ionization, Online Analysis

Characterization of a New Extractive Electrospray Ionization (EESI) Source for Online Particle Analysis and its Application to Atmospheric Aerosol

Felipe Lopez-Hilfiker[1,2], Sonja Klee[1], Manuel Hutterli[1], Veronika Pospilova[2], Jay Slowik[2]
[1]TOFWERK, Schweiz; [2]Paul Scherrer Institute (PSI), Villigen, Switzerland; klee@tofwerk.com

Poster-24-77.pdf

ID: 30 / Poster: 25
Poster
Themen: Ionisationsmethoden, Native MS
Stichworte: native MS, softness of ionization, laser desorption, energy distributions, binding affinities

Characterizing the LILBID ionization method: energy transfer and dissociation

Phoebe Young, Isabell Grübner, Genia Hense, Nina Morgner
Goethe Universität Frankfurt, Deutschland; young@chemie.uni-frankfurt.de

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ID: 127 / Poster: 26
Poster
Themen: Element- & Speziationsanalytik, Organische Massenspektrometrie
Stichworte: liquid crystal display, sealant, laser ablation, APCI-MS, ICP-MS

Analysis of Liquid Crystal Display Sealants using Spatially Resolved Mass Spectrometric Methods

Jennifer-Christin Mueller[1], Claudia Enders[2], Peter Leonhard[2], Uwe Karst[1]
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Poster-26-127.pdf

ID: 143 / Poster: 27
Poster
Themen: Element- & Speziationsanalytik, Umweltanalytik
Stichworte: ICP-MS, nanoparticles, TOF

Determination of multi-element composition and mass of single nanoparticles in liquids and air

Urs Rohner, Patrick Sturm, Olga Borovinskaya, Martin Tanner
TOFWERK, Switzerland; rohner@tofwerk.com

ID: 144 / Poster: 28
Poster
Themen: Ionisationsmethoden, Klinische Diagnostik & Forensik
Stichworte: Laser ablation, high resolution mass spectrometry, drug analysis, synthetic cannabinoids

Molecular laser ablation-mass spectrometry for rapid identification of synthetic cannabinoids

Elias Lützen[1], Uwe Karst[1], Sascha Münster-Müller[2], Michael Pütz[2]
[1]Westfählische Wilhelms-Universität Münster; [2]Bundeskriminalamt Wiesbaden; eliasluetzen@uni-muenster.de

Poster-28-144.pdf

ID: 109 / Poster: 29
Poster
Themen: Klinische Diagnostik & Forensik, Proteine & Proteomics
Stichworte: pesticides, organophosphates, mass spectrometry, biomarkers, albumin adducts

Albumin adducts as biomarkers of an exposure with organophosphorus pesticides

Jens von der Wellen, Horst Thiermann, Harald John
Bundeswehr Institute of Pharmacology and Toxicology; jensvonderwellen@bundeswehr.org

Poster-29-109.pdf

ID: 247 / Poster: 30
Poster
Themen: Klinische Diagnostik & Forensik, Proteine & Proteomics
Stichworte: Rheumatoid arthritis, mass spectrometry, oxidative stress, post translational modification

Identification of oxidative biomarkers in synovial fluid of patients suffering from rheumatoid arthritis

Dennis Westphal[1], Maria Fedorova[1,2], Ralf Hoffmann[1,2]

[1]Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig, Germany; [2]Center for Biotechnology and Biomedicine, Universität Leipzig, Germany; dennis.westphal@bbz.uni-leipzig.de

Poster-30-247.pdf

ID: 110 / Poster: 31
Poster
Themen: Klinische Diagnostik & Forensik, Proteine & Proteomics
Stichworte: Sulfur mustard, N-acetylcysteine, high-resolution mass spectrometry, scavenger, albumin adducts

Mass spectrometric investigation of N acetylcysteine as a potential scavenger against sulfur mustard

Markus Siegert[1], Horst Thiermann[2], Harald John[2]
[1]Department of Chemistry, Humboldt Universität zu Berlin, Berlin, Germany; [2]Bundeswehr Institute of Pharmacology and Toxicology, Munich, Germany; markus.siegert@student.hu-berlin.de

Poster-31-110.pdf

ID: 59 / Poster: 32
Poster
Themen: Klinische Diagnostik & Forensik, Proteine & Proteomics
Stichworte: autoimmunity, biomarker identification, MALDI-TOF mass spectrometry, immunoprecipitation

The role of mass spectrometry in the identification of autoantigens as targets in neurological autoimmune diseases

Madeleine Scharf, Ramona Miske, Stephanie Kade, Stefanie Hahn, Nora Begemann, Yvonne Denno, Christian Probst, Bianca Teegen, Kathrin Borowski, Winfried Stöcker, Lars Komorowski
Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany; n.begemann@euroimmun.de

Poster-32-59.pdf

ID: 239 / Poster: 33
Poster
Themen: Klinische Diagnostik & Forensik, Proteine & Proteomics
Stichworte: Proteomics, Protein mass spectrometric analysis, Skin, database for epidermis and dermis

Proteomic investigation of skin cell layers by tissue ablation using picosecond infrared laser (PIRL)

Parnian Kiani[1], Hartmut Schlüter[1], Jörn Hendrik Reuter[2], Tanja Bussmann[2], Nils-Owe Hansen[3], Stephanie Uschold[3], R. J. Dwayne Miller[3], Dennis Eggert[4]
[1]University Medical Centre Hamburg-Eppendorf, Institute for Clinical Chemistry, Department for Mass Spectrometric Proteomics, Hamburg; [2]Research and Development, Beiersdorf AG, Hamburg; [3]Max Planck Institute for the Structure and Dynamics of Matter CFEL, Hamburg; [4]Heinrich Pette Institute, Leibniz Institute for Experimental Virology, Hamburg; pkiani@uke.de

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ID: 99 / Poster: 34
Poster
Themen: Klinische Diagnostik & Forensik, Metaboliten & Metabolomics
Stichworte: N-Acetyltaurine, Taurine, Alcohol marker, Abstinence monitoring, Urine analysis, LC-MS/MS

N-Acetyltaurine as a novel urinary ethanol marker in a drinking study

Marc Luginbühl[1], Sofie Rutjens[2], Stefan Koenig[1], Julien Furrer[3], Wolfgang Weinmann[1]
[1]Institute of Forensic Medicine, University of Bern; [2]Laboratory of Toxicology, University of Ghent; [3]Department of Chemistry and Biochemistry, University of Bern; marc.luginbuehl@irm.unibe.ch

Poster-34-99.pdf

ID: 214 / Poster: 35
Poster
Themen: Klinische Diagnostik & Forensik, Sonstiges
Stichworte: Explosives, HPLC, HR-MS

Differentiation and Identification of Explosives Formulations by Means of HPLC-MS

Tilo D. Schachel, Uwe Karst
Westfälische Wilhelms-Universität Münster, Deutschland; tilo.schachel@uni-muenster.de

Poster-35-214.pdf

ID: 212 / Poster: 36
Poster
Themen: Ionenmobilität, Klinische Diagnostik & Forensik
Stichworte: tetrahydrocannabinol, cannabidiol, marijuana, ion mobility-MS, forensic chemistry

Separation of isomeric cannabinoids by high-resolution ion mobility-MS for the differentiation of legal and illegal marijuana

Marianne Hädener[1], Wolfgang Weinmann[1], Michael Groessl[2]
[1]University of Bern, Institute of Forensic Medicine, Forensic Toxicology and Chemistry, Bühlstrasse 20, 3012 Bern, Switzerland; [2]TOFWERK, Uttigenstrasse 22, 3600 Thun, Switzerland; marianne.haedener@irm.unibe.ch

Poster-36-212.pdf

ID: 241 / Poster: 37
Poster
Themen: Instrumentelle Entwicklungen, Klinische Diagnostik & Forensik
Stichworte: DSA, TOF, LC, Screening

Rapid Screening of Methylamphetamine in Hair of Drug Addicts using DSA-TOF

Stefan Edler
LAS Perkinelmer GmbH, Deutschland; stefan.edler@perkinelmer.com

Poster-37-241.pdf

ID: 248 / Poster: 38
Poster
Themen: Instrumentelle Entwicklungen
Stichworte: mass spectrometry, instrumentation, single particle analysis, delayed ion extraction

Optimization of the LAMPAS 3 laser mass spectrometer for improved on-line single particle analysis

Klaus-Peter Hinz, Christof Barth, Bernhard Spengler
Justus-Liebig-Universität Gießen, Deutschland; Klaus-Peter.Hinz@anorg.Chemie.uni-giessen.de

Poster-38-248.pdf

ID: 131 / Poster: 39
Poster
Themen: Instrumentelle Entwicklungen
Stichworte: tandem mass spectrometry, time of flight, high resolving power, high separation power

Tandem Mass Spectrometry with a (Ultra-)High Resolving Time-of-Flight Mass Spectrometer

Julian Bergmann[1], Wayne Lippert[1], Johannes Lang[1], Timo Dickel[1,2], Wolfgang R. Plaß[1,2], Hans Geissel[1,2], Christoph Scheidenberger[1,2], Mikhail Yavor[3], Alexander Pikhtelev[4], Samuel Ayet San Andrés[1,2]
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Poster-39-131.pdf

ID: 83 / Poster: 40
Poster
Themen: Instrumentelle Entwicklungen
Stichworte: Field ionisation, FI, GCMS, molecular weight determination

Field ionization: an old but still useful method

Christian Bartelmus, Sophie Brogly, Oliver Scheidegger
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ID: 218 / Poster: 41
Poster
Themen: Instrumentelle Entwicklungen, Umweltanalytik
Stichworte: on site analysis, portable GC/MS

Rapid On Site Analysis of BTX with Portable GC/MS

Martin Dinse, Alan Gallaspy, Bill Hahn, Charlie Schmidt
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ID: 250 / Poster: 42
Poster
Themen: Instrumentelle Entwicklungen, Ionisationsmethoden

Stichworte: Single particle aerosol mass spectrometry, ATOFMS, laser desorption–laser post ionization, LDI polycyclic aromatic hydrocarbons, inorganic core

Multiple analysis of individual airborne aerosol particles by laser mass spectrometry: Detection of polyaromatic hydrocarbons from the particle-surface and particle-core

Johannes Passig[1], Julian Schade[1], M. Fuchs[2], M. Oster[2], Martin Sklorz[1], Ralf Zimmermann[1,2]
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Poster-42-250.pdf

ID: 124 / Poster: 43
Poster
Themen: Instrumentelle Entwicklungen
Stichworte: Photoionisation, Fuel Characterisation, Thermal Analysis

Thermogravimetry coupled to Ultrafast Gas Chromatography Singlephoton-Ionisation Time-of-Flight-Mass-Spectrometry (TG-SPI-TOF-MS) for Evolved-Gas-Analysis of Fuels regarding to the Deposit Formation Potential

Anne Ulbrich[1], Winfried Koch[2], Sebastian Wohlfahrt[3], Michael Fischer[3], Thorsten Streibel[1,3], David Diarra[2], Ralf Zimmermann[1,3]
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Poster-43-124.pdf

ID: 179 / Poster: 44
Poster
Themen: Instrumentelle Entwicklungen, Ionisationsmethoden
Stichworte: Single-photon ionization, SALDI, elevated pressure ion source, oMALDI2, laser mass spectrometry

Single-photon ionization of laser desorbed molecules in a fine-vacuum ion source

Christoph H. M. Bookmeyer[1], Andreas Schnapp[1], Klaus Dreisewerd[1,2]
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ID: 217 / Poster: 45
Poster
Themen: Instrumentelle Entwicklungen, Native MS
Stichworte: Antibodies, Biopharmaceuticals, Native MS, high mass range

Full Characterization of Antibodies Under Denaturing and Native Conditions on a Hybrid Quadrupole-Orbitrap MS Equipped With a Higher Mass Range

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Poster-45-217.pdf

ID: 111 / Poster: 46
Poster
Themen: Instrumentelle Entwicklungen, Lipide & Lipidomics
Stichworte: Lipidomics, DIQ, new data independent acquisition method

Lipidomics Quantitation Using a Novel Scanning Quadrupole DIA Method

Gunnar Weibchen[1], Chris Hughes[2], Keith Richardson[2], Jason Wildgoose[2], Lee Gethings[2], James Langridge[2]
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Poster-46-111.pdf

ID: 240 / Poster: 47
Poster
Themen: Instrumentelle Entwicklungen, Umweltanalytik
Stichworte: high resolution mass spectrometry, evolved gas analysis, atmospheric pressure ionisation, thermal desorption, laser desorption

Thermal and laser desorption atmospheric pressure photo ionisation ultra high resolution mass spectrometry – Concept and application towards complex samples

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Poster-47-240.pdf

ID: 35 / Poster: 48
Poster
Themen: Instrumentelle Entwicklungen, Proteine & Proteomics
Stichworte: SONAR, Quantification, Proteomics, DIA, Scanning

Quantitation of Proteomics Samples Using a Novel Scanning Quadrupole DIA Method

Marc Kipping[1], Chris Hughes[2], Keith Richardson[2], Jason Wildgoose[2], Lee Gethings[2], James Langridge[2], John Hoyes[2], Johannes PC Vissers[2]
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ID: 46 / Poster: 49
Poster
Themen: Instrumentelle Entwicklungen, Ionisationsmethoden
Stichworte: Ambient mass spectrometry, Ionization, Emission spectroscopy, Laser induced plasma, High repetition rate laser

Improving the performance of the airborne laser-spark ion source for the detection of volatile organic compounds under ambient conditions

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Poster-49-46.pdf

ID: 174 / Poster: 50
Poster
Themen: Instrumentelle Entwicklungen
Stichworte: trapped ion mobility ms

High resolution trapped ion mobility mass spectrometry analysis of isomeric compounds

Sven W. Meyer, Ulrike Burmester
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ID: 172 / Poster: 51
Poster
Themen: Instrumentelle Entwicklungen
Stichworte: Direct Inlet Probe, Time-of-flight MS, High Resolution MS

The Usage of Direct Inlet Probe in combination with High Resolution Mass Spectrometry

Juergen Wendt[1], Uwe Kaefer[2]
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ID: 66 / Poster: 52
Poster
Themen: Instrumentelle Entwicklungen, Ionenmobilität
Stichworte: IR-MALDI, ion mobility, structure, peptides, collision cross-sections

IR-MALDI Ion Mobility Spectrometry: Low and High Field Mobilities of Peptide Ions at Intermediate Pressure

José Villatoro[1,3,4], Daniel Riebe[1], Toralf Beitz[1], Marcus Weber[2], Hans-Gerd Löhmannsröben[1]
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Poster-52-66.pdf

ID: 56 / Poster: 53
Poster
Themen: Instrumentelle Entwicklungen, Native MS
Stichworte: LILBID QTOF, Native Mass Spectrometry, Protein net charge

Monitoring and correlating of protein charge states with respect to amino acid modification and buffer conditions

Kudratullah Karimi, Jan Hoffmann, Nils Hellwig, Nina Morgner
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Poster-53-56.pdf

ID: 45 / Poster: 54
Poster
Themen: Lipide & Lipidomics
Stichworte: UV-LDI-MS, lipids, double bond position, ozonolysis, MS/MS

Elucidation of double bond positions in lipids by means of off-line ozonolysis followed by ultraviolet laser desorption ionization mass spectrometry

Eike Ulrich Brockmann[1], Andreas Schnapp[1], Klaus Dreisewerd[1,2]
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ID: 168 / Poster: 55
Poster
Themen: Lipide & Lipidomics
Stichworte: Lipidomics, Fatty acid metabolism, Proteomics

SIMPLEX reveals myoglobin as a key player in cardiac lipid metabolism

Cristina Coman[1], Ulrike B. Hendgen-Cotta[2], Sonja Esfeld[2], Robert Ahrends[1], Matthias Totzeck[2]
[1]Leibniz-Institut für Analytische Wissenschaften – ISAS e.V., Germany; [2]University Hospital Essen, Medical Faculty, West German Heart and Vascular Center, Department of Cardiology and Department of Angiology, Germany; cristina.coman@isas.de

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ID: 238 / Poster: 56
Poster
Themen: Lipide & Lipidomics
Stichworte: PIRL, DIVE, Lipids, DDA

Lipidomics of Pig Brain Using the PIRL-DIVE Homogenisation Technique

Marceline Manka Fuh[1], Marcus Wurlitzer[1], Dominik Schwudke[2], Nils-Owe Hansen[3], Dwayne Miller[3], Hartmut Schlüter[1]
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Poster-56-238.pdf

ID: 141 / Poster: 57
Poster
Themen: Lipide & Lipidomics
Stichworte: UPLC-MS/MS, diacyl-glycerophospholipids, negative ion ESI, structural isomer mixtures

Spotting of Structural Isomer Mixtures of Diacyl-Glycerophospholipids via UPLC-MS/MS

Wolf-Dieter Lehmann[1,2], Katharina Wozny[2], Britta Brügger[2]
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Poster-57-141.pdf

ID: 114 / Poster: 58
Poster
Themen: Lipide & Lipidomics
Stichworte: Brustkrebszellen, HILIC, Phospholipide, Lipidprofiling, BMP

Profiling von konfigurationsisomeren Phospholipiden mittels HILIC-ESI-MS/MS

Christian Vosse, Heiko Hayen
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Poster-58-114.pdf

ID: 50 / Poster: 59
Poster
Themen: Ionenmobilität, Lipide & Lipidomics
Stichworte: Detergens removal, Lipidomics, SelexIon

SelexION® DMS-based detergent interference removal for shotgun-lipidomics analyses

Cyrus Papan[1], Julian Langer[2]
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Poster-59-50.pdf

ID: 102 / Poster: 60
Poster
Themen: Lipide & Lipidomics
Stichworte: Lipidanalytik, Doppelbindungsposition, Paternò Büchi Reaktion

Bestimmung von Doppelbindungspositionen in Lipiden mittels photochemischer Nachsäulenderivatisierung und Tandem-MS

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Poster-60-102.pdf

ID: 126 / Poster: 61
Poster
Themen: Lipide & Lipidomics
Stichworte: electrochemical oxidation, mass spectrometry detection, lipid oxidation

In situ monitoring of lipid oxidation using electrochemistry-mass spectrometry coupling

Giulia Coliva[1,2], Simone Colombo[3], Agnieszka Kraj[4], Jean-Pierre Chervet[4], M. Rosario Domingues[3], Pedro Domingues[3], Maria Fedorova[1,2]
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Poster-61-126.pdf

ID: 159 / Poster: 62
Poster
Themen: Metaboliten & Metabolomics
Stichworte: human endogenous metabolites

Enabling High-Confidence Human Endogenous Metabolite Identification via High-Resolution MS/MS Retention-Time Library

Nan Wang[1], Stephan Kühne[2], Aiko Barsch[2], Ulrike Schwaiger-Hufnagel[2], Xian Luo[1], Shuang Zhao[1], Yiman Wu[1], Zhendong Li[1], Wei Han[1], Jaspaul Tatlay[1], Yunong Li[1], Kevin Hooton[1], Dorothea Mung[1], Adriana Buzatto[1], Xiaohang Wang[1], Liang Li[1]
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ID: 157 / Poster: 63
Poster
Themen: Metaboliten & Metabolomics
Stichworte: LC-HRAM-MS/MS

Boosting compound identification confidence in Metabolomics by exploiting all available Q-TOF high resolution accurate mass spectral information.

Nikolas Kessler[1], Stephan Mävers[1], Frederik Walter[2], Marcus Persicke[2], Jörn Kalinowski[2], Matthias Szesny[1], Aiko Barsch[1], Heiko Neuweger[1]
[1]Bruker Daltonik GmbH, Deutschland; [2]Bielefeld University, Bielefeld, Deutschland; Matthias.szesny@bruker.com

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ID: 94 / Poster: 64
Poster
Themen: Metaboliten & Metabolomics
Stichworte: N-acyl homoserine lactones, quorum sensing, microscale synthesis, ionic liquid matrices, MALDI MS

Identification and quantification of N-acyl homoserine lactones involved in bacterial communication by matrix-assisted laser desorption/ionization mass spectrometry

Jan Leipert, Christian Treitz, Andreas Tholey
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ID: 119 / Poster: 65
Poster
Themen: Metaboliten & Metabolomics
Stichworte: PIRL, Metabolomics, LC-MS/MS, FIA-MS/MS

Application of laser ablation for tissue metabolomics

Jonas Klein[1], Laura Heikaus[1], Gerrit Wolters-Eisfeld[1], Thomas Benninghaus[1], Nils-Owe Hansen[2], Dwayne Miller[2], Hartmut Schlüter[1]
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ID: 1 / Poster: 66
Poster
Themen: Metaboliten & Metabolomics, Organische Massenspektrometrie
Stichworte: Turnover of photopigments, 13C labelling, LC-MS, FTICR-MS

Quantitative turnover analysis of chlorophylls, carotenoids and tocopherol in green leaves by LC-MS and FTICR-MS

Björn Thiele, Andrea Neuwohner, Siegfried Jahnke, Ingar Janzik, Shizue Matsubara
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Poster-66-1.pdf

ID: 78 / Poster: 67
Poster
Themen: Metaboliten & Metabolomics, Organische Massenspektrometrie
Stichworte: phlorotannins, brown algae, LC-MS

Application of LC-MS technique for intra-thallus profiling of polyphenolics in three species of fucoid algae

Valeriia Lemesheva[1], Claudia Birkemeyer[2], Elena Tarakhovskaya[1]
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Poster-67-78.pdf

ID: 41 / Poster: 68
Poster
Themen: Metaboliten & Metabolomics, Sonstiges
Stichworte: Metabolomics, Chemical Profiling of Plant Extracts, Genotypes, Actaea racemosa

UPLC-ESI-QTOF-MS based chemical profiling of Actaea racemosa L. (black cohosh) rhizomes to investigate differences in cultivation, wild harvest, and genotypes

Marian Bittner[1], Andreas Springer[2], Regina Schenk[3], Matthias F. Melzig[1]
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Poster-68-41.pdf

ID: 158 / Poster: 69
Poster
Themen: Metaboliten & Metabolomics
Stichworte: MS based metabolite profiling strategies, metabolites, insects

Metabolomics to study the "war" between plants and insects - Systemic defense induction and post-ingestive rearrangement of plant toxins in insects.

Sven Heiling[1], Emmanuel Gaquerel[2], Aiko Barsch[3], Heiko Neuweger[3], Matthias Szesny[3], Ian T. Baldwin[1]
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ID: 156 / Poster: 70
Poster
Themen: Metaboliten & Metabolomics
Stichworte: Metabolomics

A step forward in GC-HRAM-MS based metabolomics - A novel atmospheric pressure GC-APCI Source increases quantitative and qualitative performance

Christian J. Wachsmuth[1], Aiko Barsch[2], Stephan Kühne[2], Peter J. Oefner[1], Katja Dettmer[1]

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ID: 209 / Poster: 71
Poster
Themen: Metaboliten & Metabolomics, Lebensmittelanalytik
Stichworte: Metabolomic Fingerprinting, Food Authenticity, UPLC-IMS-QToF, Foodomics

Discrimination of apple and potato cultivars by non-targeted metabolomic fingerprinting via UPLC-IMS-QToF analysis

Christin Claassen[1], Jasmin Wrage[1], Sascha Rohn[2], Jürgen Kuballa[1]
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Poster-71-209.pdf

ID: 128 / Poster: 72
Poster
Themen: Metaboliten & Metabolomics, Umweltanalytik
Stichworte: GC-MS, Metabolites, Anaerobic bio-degradation, Phenanthrene, TRIP

Metabolite analysis of the phenanthrene degrading, sulfate reducing bacterial enrichment culture (TRIP) using GC-MS

Zahra Farmani[1,2], Rainer U. Meckenstock[1], Wolfgang Schrader[2]
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Poster-72-128.pdf

ID: 82 / Poster: 73
Poster
Themen: Metaboliten & Metabolomics, Lebensmittelanalytik
Stichworte: Miniature mass spectrometry, food analysis, authentication, principal component analysis

Real-time food authentication with a miniature mass spectrometer

Stefanie Gerbig, Stephan Neese, Alexander Penner, Bernhard Spengler, Sabine Schulz
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Poster-73-82.pdf

ID: 148 / Poster: 74
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging, MS - Informatik / Bioinformatik
Stichworte: imzML, Mass spectrometry imaging, MSI visualization tools, converters, public data repository

Overview of imzML-based software tools for MS imaging

Amol Fatangare, Nicolas Desbenoit, Andreas Römpp
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ID: 122 / Poster: 75
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging, Lipide & Lipidomics
Stichworte: MALDI MSI, Phospholipids, Ion suppression

Micro-arrays of faux tissue to investigate ion suppression effects in MALDI mass spectrometry of lipids

Marcel Boskamp[1], Fabian Eiersbrock[1], Marcel Wiegelmann[1], Klaus Dreisewerd[1,2], Jens Soltwisch[1,2]
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ID: 199 / Poster: 76
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging, Instrumentelle Entwicklungen
Stichworte: MALDI FT-ICR Imaging

MALDI FT-ICR Imaging: Double the Performance or Double the Samples using Quadrupolar Detection

Shannon Cornett[1], Christopher Thompson[1], Roland Jertz[3], Christoph Goseli[2], Claudia Kriete[3], Jochen Friedrich[3], Matthias Witt[3], Steve VanOrden[1], Michael Easterling[1], Christian Berg[1], Eugene Nikolaev[4], Arndt Asperger[3], Gökhan Baykut[3]

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ID: 194 / Poster: 77
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging
Stichworte: MRI contrast agents, mass spectrometry imaging, biological tissues

Mass Spectrometry Imaging as Tool for the Analysis of MRI Contrast Agents in Biological Tissues

Sabrina Trog[1], Ahmed El-Khatib[1], Hee-Jin Lee[1], Marcus R. Makowski[2], Sebastian Beck[1], Norbert Jakubowski[3], Michael W. Linscheid[1]
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Poster-77-194.pdf

ID: 234 / Poster: 78
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging, Proteine & Proteomics
Stichworte: DIVE, PIRL, laser ablation, proteome analysis, cell lysate collection

Optimized Biomolecular Extraction Using Desorption by Impulsive Vibrational Excitation: Applications to Embryonic Cell Differentiation

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ID: 232 / Poster: 79
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging, Instrumentelle Entwicklungen
Stichworte: mass spectrometry imaging, laser desorption ionization, infrared laser desorption

Development of Sub-Cellular Mass Spectrometry Imaging by Impulsive IR Laser Ablation

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ID: 89 / Poster: 80
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging, Lipide & Lipidomics
Stichworte: MALDI-MSI, Lipidomics, Ionion suppression, MALDI-2

Towards qMALDI-MSI : MS imaging of phospholipids in mouse cerebellum followed by semi-quantitative nano-HPLC-ESI-MS of extracts from laser micro-dissected brain regions

Fabian Eiersbrock[1], Marcel Boskamp[1], Michael Mormann[1], Klaus Dreisewerd[1,2], Jens Soltwisch[1]
[1]Institute for Hygiene, University of Münster, Germany; [2]Interdisciplinary Center for Clinical Research (IZKF), University of Münster, Germany; f_eier01@wwu.de

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ID: 29 / Poster: 81
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging, Proteine & Proteomics
Stichworte: LA-ICP-MS, SDS-PAGE, Internal Standard, MeCAT

A new internal standard approach for laser ablation ICP-MS of polyacrylamide gels

René Becker, Jule Heimerl, Ahmed El-Khatib, Michael W. Linscheid
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Poster-81-29.pdf

ID: 136 / Poster: 82
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging, MS - Informatik / Bioinformatik
Stichworte: MALDI Imaging, Raman Imaging, MS/Raman Data processing, imzML

Multimodal imaging combining mass spectrometry and vibrational spectroscopy using a single tissue section and an integrated data processing workflow

Rico Scheier, Nicholas Desbenoit, Axel Treu, Jasmin Kniese, Julia Kokesch-Himmelreich, Heinar Schmidt, Andreas Römpp

Universität Bayreuth, Deutschland; Axel.Treu@uni-Bayreuth.de

Poster-82-136.pdf

ID: 25 / Poster: 83
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging, Lebensmittelanalytik
Stichworte: MALDI-MSI, MS Imaging, Sclerotia, Mycotoxins, Ergot alkaloids

Localization of Ergot Alkaloids in Sclerotia of Claviceps purpurea by MALDI-MS Imaging

Simeon Vens-Cappell[1,2], Julian Dopstadt[3], Lisa Neubauer[4], Paul Tudzynski[4], Benedikt Cramer[3], Klaus Dreisewerd[1,2], Hans-Ulrich Humpf[3]
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ID: 100 / Poster: 84
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging, Instrumentelle Entwicklungen
Stichworte: MALDI-MSI, IR-MALDI, Postionization, Metabolites

CoolMALDI: Combination of IR-ablation and UV-postionization of snap-frozen tissue sections for sensitive imaging of lipids and metabolites

Jens Soltwisch[1,2], Hans Kettling[1,2], Simeon Vens-Cappell[1,2], Klaus Dreisewerd[1,2]
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ID: 96 / Poster: 85
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging
Stichworte: superbasic matrix DPN, AP-MALDI, AP-SMALDI-FT MSI, lipids, glucosinolates

Application of the Superbasic Matrix DPN in Atmospheric Pressure MALDI-MS-Analyses of Biological Samples

Jerrit Weissflog[1], Filip Kaftan[1], Aleš Svatoš[1,2]
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Poster-85-96.pdf

ID: 24 / Poster: 86
Poster
Themen: Sonstiges
Stichworte: Tandem MS, Oligonucleotides

Collision Specific Fragmentation of Oligonucleotides in Tandem Mass Spectrometry Experiments

Stefanie Ickert[1], Jens Riedel[1], Sebastian Beck[2], Michael Linscheid[2]
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Poster-86-24.pdf

ID: 15 / Poster: 87
Poster
Themen: Sonstiges
Stichworte: Pyridinderivate, REMPI-Spektroskopie, MATI-Spektroskopie, Anregungsenergien, Ionisationsenergien

REMPI- und MATI-Spektroskopie an den Methylpyridinen

Niklas Helle, Sascha Krüger, Jürgen Grotemeyer
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Poster-87-15.pdf

ID: 185 / Poster: 88
Poster
Themen: Sonstiges
Stichworte: ultra High Throughput Screening

Ultra High Throughput Drug Discovery Screening by MALDI-TOF Mass Spectrometry

Carl Haslam[1], Peter Marshall[1], Neil Hardy[1], Melanie Leveridge[1], Adrian Dunn[1], Meike Hamester[2], Jens Fuchser[2], Arne Fuetterer[2], Volker Sauerland[2], Arndt Asperger[2], Adrian Siemers[3], Swen Tyrasa[3], Debra Conway[3]
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ID: 151 / Poster: 89
Poster
Themen: Sonstiges
Stichworte: volatile analysis, mobile mass spectrometry, body odour sampling

The performance of mobile GC-MS for field sampling of body odours from common marmosets (Callithrix jacchus)

Marlen Kücklich[1], Manfred Möller[2], Andrea Marcillo[1], Almuth Einspanier[1], Anja Widdig[1,3,4], Claudia Birkemeyer[1]
[1]Universität Leipzig, Deutschland; [2]Uniklinik der RWTH Aachen, Deutschland; [3]Max-Planck-Institut für Evolutionäre Anthropologie, Leipzig, Deutschland; [4]Deutsches Zentrum für integrative Biodiversitätsforschung, Leipzig, Deutschland; birkemeyer@chemie.uni-leipzig.de

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ID: 118 / Poster: 90
Poster
Themen: Glyco-Analytik & Glycomics, Native MS
Stichworte: Glycan analysis, middle down proteomics, In-Source-Fragmentation, Quantification

Analysis of human Glycoproteins with different LC-MS/MS and NMR techniques

Melissa Bärenfänger, Bernd Meyer
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Poster-90-118.pdf

ID: 87 / Poster: 91
Poster
Themen: Glyco-Analytik & Glycomics, Proteine & Proteomics
Stichworte: N-glycosylation, heterologous expression, nanoESI MS, CID

Identification of an unusual N-glycan detected in a tryptic glycopeptide derived from intergrin α7 expressed in Drosophila S2 cells

Julius Grosche[1], Johannes Eble[1], Michael Mormann[2], Gottfried Pohlentz[2]
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Poster-91-87.pdf

ID: 177 / Poster: 92
Poster
Themen: Glyco-Analytik & Glycomics, Proteine & Proteomics
Stichworte: O-glycosylation, GalNAc, VVA, enrichment

Mass spectrometric characterization of aberrant O-glycosylation in COSMC deficient mouse pancreas tissue

Benjamin Dreyer, Dennis Krösser, Pascal Steffen, Baris Mercanoglu, Gerrit Wolters-Eisfeld, Hartmut Schlüter
University Medical Center Hamburg Eppendorf, Deutschland; b.dreyer@uke.de

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ID: 101 / Poster: 93
Poster
Themen: Ionenmobilität, Glyco-Analytik & Glycomics
Stichworte: N-linked glycopeptides, N-linked glycoproteins

Increased confidence for the identification of N-linked glycopeptides using an optimised collision energy workflow

Gunnar Weibchen[1], Yi J Chen[2], Lee A Gethings[3], Alex Kuo[2], Yu-Ju Chen[2]
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Poster-93-101.pdf

ID: 166 / Poster: 94
Poster
Themen: MS - Informatik / Bioinformatik, Metaboliten & Metabolomics
Stichworte: HPLC, high resolution mass spectrometry, Metabolomics, MZmine 2, Algorithm

Algorithms for the annotation of isotopes, fragments and adducts, applied to HPLC-HRMS metabolomics data for the discovery of novel compounds

Robin Schmid[1,2], **Birgit Arndt**[1], **Florian Hübner**[1], **Uwe Karst**[2], **Hans-Ulrich Humpf**[1]
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Poster-94-166.pdf

ID: 167 / Poster: 95
Poster
Themen: MS - Informatik / Bioinformatik, Proteine & Proteomics
Stichworte: AGEs, GC-MS, glycation, metabolomics, microgravity, oxidative stress, seed germination, tandem mass spectrometry.

Simulated microgravity triggers transient enhancement of protein glycation and oxidation in germinating Brassica napus seeds

Veronika Chantseva[1], **Anna Didio**[2,3], **Christian Ihling**[4], **Rico Schmidt**[4], **Galina Smolikova**[1], **Tatyana Grishina**[3], **Wolfgang Hoehenwarter**[5], **Andrej Frolov**[2], **Andrea Sinz**[4], **Sergei Medvedev**[1], **Tatiana Bilova**[1,2]
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Poster-95-167.pdf

ID: 117 / Poster: 96
Poster
Themen: MS - Informatik / Bioinformatik, Proteine & Proteomics
Stichworte: bone healing, glycosaminoglycans, random forest modelling, SILAC

Comparative analysis of the effects of sulfated hyaluronic acid and dexamethasone on osteoblast differentiation by nanoLC-MS and random forest modeling.

Johannes R. Schmidt[1], **Sarah Vogel**[2], **Stefan Kalkhof**[3], **Stephanie Möller**[4], **Martin von Bergen**[1,5], **Ute Hempel**[2]
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Poster-96-117.pdf

ID: 147 / Poster: 97
Poster
Themen: MS - Informatik / Bioinformatik, Proteine & Proteomics
Stichworte: AGEs, aging, glycation, mass spectrometry, nodule, Phaseolus vulgaris, plant-microbial interaction, proteomics

Age-related formation of advanced glycation end products (AGEs) in root nodules of common beans (Phaseolus vulgaris)

Ahyoung Kim[1,2], **Tatiana Bilova**[1], **Christian Ihling**[3], **Manuel Matamoros**[4], **Manuel Becana**[4], **Andrea Sinz**[3], **Ludger A. Wessjohann**[1], **Andrej Frolov**[1]
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Poster-97-147.pdf

ID: 69 / Poster: 98
Poster
Themen: MS - Informatik / Bioinformatik
Stichworte: Elemental composition, accurate mass, isotope pattern

Determination of Molecular Formulas from Complex Isotope Pattern

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ID: 233 / Poster: 99
Poster
Themen: MS - Informatik / Bioinformatik, Proteine & Proteomics
Stichworte: Orbitrap, MS-cleavable cross-linkers

Optimization of crosslinked peptide analysis on an Orbitrap Fusion Lumos mass spectrometer

Ryan Bomgarden[1], Erum Raja[1], Chris Etienne[1], Fan Liu[4], Albert Heck[4], Mathias Müller[2], Rosa Viner[3]
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ID: 36 / Poster: 100
Poster
Themen: Ionenmobilität, Proteine & Proteomics
Stichworte: IMS, MRM, QconCAT, Proteomics, Lipidomics

IMS-DIA-MS Characterisation and IMS-MRM QconCAT Quantitation of the Lipidome and Apolipoprotein Complements of Obesity and Diabetes Cohorts

Marc Kipping[1], Lee A Gethings[2], Johannes PC Vissers[2], Jose Castro-Perez[3], Yvonne Woolerton[4], Lynn McLean[4], Robert Beynon[4], James Langridge[2]
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ID: 49 / Poster: 101
Poster
Themen: Ionenmobilität, Metaboliten & Metabolomics
Stichworte: derivatization, headspace gas chromatography, ion-mobility spectrometry, metabolomic fingerprinting

Derivatization of low-volatile compounds in aqueous solution and analysis by HS-GC-IMS

Alexander Roth, Fabian Simon, Vanessa König, Philipp Weller
Hochschule Mannheim, Deutschland; rotha@hs-mannheim.de

Poster-101-49.pdf

ID: 67 / Poster: 102
Poster
Themen: Ionenmobilität, Native MS
Stichworte: LILBID-MS, nESI, Ion Mobility, ATPase, ABC Transporter

Analyzing macromolecular complexes: subunit interactions of the F1F0 ATP synthase and conformational changes of the heterodimeric ABC transport complex TmrAB

Khanh Vu Huu, Stefan Brüchert, Robert Tampé, Volker Müller, Nina Morgner
Johann Wolfgang Goethe-Universität, Deutschland; VuHuu@chemie.uni-frankfurt.de

Poster-102-67.pdf

ID: 64 / Poster: 103
Poster
Themen: Ionenmobilität
Stichworte: Ion Mobility-Mass Spectrometry, Gas-Phase IR Spectroscopy, Human Islet Amyloid Polypeptide, Amyloid Intermediates

The Amyloid Formation Mechanism of Human IAPP: An Infrared Spectroscopy Approach

Waldemar Hoffmann[1], Michael T. Bowers[2], Gert von Helden[3], Kevin Pagel[1]
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ID: 28 / Poster: 104
Poster
Themen: Ionenmobilität, Lebensmittelanalytik
Stichworte: Authenticity assessment, Fingerprinting, Multivariate data analysis

Quality assessment of olive oil based on volatile compound fingerprinting using HRGC-IMS analysis

Natalie Gerhardt[1], Sascha Rohn[2], Philipp Weller[1]
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Poster-104-28.pdf

ID: 201 / Poster: 105
Poster
Themen: Organische Massenspektrometrie, Sonstiges
Stichworte: ageing, charcoal, extract, ESI-FTICRMS, soil

Historical charcoal additions potentially improve stability of soil organic carbon

Diana Hofmann[1], Bernhard Steffen[1], Hamada Abdelrahman[2], Ulrich Disko[1], Nele Meyer[3], Nils Borchard[4]
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Poster-105-201.pdf

ID: 6 / Poster: 106
Poster
Themen: Organische Massenspektrometrie, Sonstiges
Stichworte: MALDI-TOF-MS, Jeffamine, exakte Masse, Massenkalibrierung, Summenformel

Evaluierung basischer Polypropylenglycole als Standards zur internen Kalibrierung für exakte Massen in der positiv-Ionen MALDI-TOF-MS

Jürgen Gross
Universität Heidelberg, Deutschland; juergen.gross@oci.uni-heidelberg.de

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ID: 237 / Poster: 107
Poster
Themen: Organische Massenspektrometrie
Stichworte: MALDI-MS, MALDI matrix, small molecules

CICCA-Tetrazole: An alternative matrix for the analysis of low molecular weight compounds by MALDI-MS

Anne Arnold, Michael Rühl, Michael Karas
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ID: 116 / Poster: 108
Poster
Themen: Organische Massenspektrometrie
Stichworte: Metaorganism, N-acyl homoserine lactone, quorum-sensing, quorum-quenching

Identification and characterization of N-acyl homoserine lactones by mass spectrometry

Christian Treitz[1], Cleo Pietschke[2], Sebastian Fraune[2], Andreas Tholey[1]
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ID: 221 / Poster: 109
Poster
Themen: Lebensmittelanalytik, Organische Massenspektrometrie
Stichworte: LC-MS/MS, Combined Fast Mode, Polarity Switching, Vitamins, Nutritional Supplements

Combined Fast Mode and Polarity Switching for Analysis of a Range of Vitamins and Nutritional Supplements in a Single Injection

Volker Heber
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ID: 140 / Poster: 110
Poster
Themen: Lebensmittelanalytik, Organische Massenspektrometrie
Stichworte: Muscarine, normuscarine, diastereomeric separation, enantiomeric separation

Separation and identification of muscarine isomers

Axel Treu[2], Thomas Dülcks[1], Peter Spiteller[1]
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Poster-110-140.pdf

ID: 17 / Poster: 111
Poster
Themen: Lebensmittelanalytik
Stichworte: SFE, SFC, LC-MS, GC-MS

Analysis of pesticides in food product using SFE-SFC-MSMS

Davor Fielitz[1], Sigrid Baumgarten[2]
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Poster-111-17.pdf

ID: 60 / **Poster: 112**
Poster
Themen: Lebensmittelanalytik
Stichworte: Folate, Stabilisotopenverdünnungsanalyse, LC-MS/MS, Validierung, Lebensmittel

Validierung einer Stabilisotopenverdünnungsanalyse von Folaten in Lebensmitteln und Bestimmung des Folatgehaltes in Naturprodukten

Nina Firl[1], Lisa Striegel[2], Christian Bunse[1], Michael Rychlik[2]
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Poster-112-60.pdf

ID: 155 / **Poster: 113**
Poster
Themen: Umweltanalytik, Lebensmittelanalytik
Stichworte: Environmental Contaminants

Simultaneous quantitation and confirmation of about 500 pesticide residues in food extracts using LC-QTOF accurate mass spectrometry

Petra Decker, Jochen Boosfeld, Karin Wendt, Carsten Baesmann
Bruker Daltonik GmbH, Deutschland; jochen.boosfeld@bruker.com

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ID: 188 / **Poster: 114**
Poster
Themen: Umweltanalytik
Stichworte: multiple polar pesticides

Parts-per-trillion level high-throughput quantitation of glyphosate, aminomethylphosponic acid (AMPA) and glufosinate in water samples by LC-MS/MS

Javier Lopez[1], Diego Martin[1], Cesar Perez[1], Jochen Boosfeld[2]
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ID: 230 / **Poster: 115**
Poster
Themen: Umweltanalytik
Stichworte: Fouier transform Orbitrap mass spectrometry, supercritical fluid extraction, crude oil, soil remediation

Supercritical fluid extraction as a soil remediation method for removal of crude oil related contaminations, analyzed by FT Orbitrap MS

Ruoji Luo, Wolfgang Schrader
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Poster-115-230.pdf

ID: 190 / **Poster: 116**
Poster
Themen: Umweltanalytik
Stichworte: VOCs, thermal desorption, GC-MS, XAD-2

Methodological aspects of mass spectrometric detection for profiling ambient VOCs with thermodesorption-GCMS

Andrea Marcillo[1], Arne Koch[1], Ilya Kozlov[1], Viktorija Jakimovska[4], Anja Widdig[1,2,3], Claudia Birkemeyer[1]
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Poster-116-190.pdf

ID: 165 / **Poster: 117**
Poster
Themen: Umweltanalytik, Sonstiges
Stichworte: Crude oil, Fenton reaction, supercritical CO2, Fourier transform Orbitrap mass spectrometry

Fenton based oxidation of crude oil in supercritical CO2

Ilker Satilmis, Wolfgang Schrader
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Poster-117-165.pdf

ID: 197 / Poster: 118
Poster
Themen: Umweltanalytik, Organische Massenspektrometrie
Stichworte: Crude oil, fouling, ESI

Effect of temperature on crude oil fouling under inert and oxygenated conditions and subsequent analysis by HRMS

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Poster-118-197.pdf

ID: 183 / Poster: 119
Poster
Themen: Umweltanalytik, Organische Massenspektrometrie
Stichworte: Sulfamethoxazole, AOPs, photolysis, LC-HRMS

Investigations on the photolysis of sulfamethoxazole

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Poster-119-183.pdf

ID: 55 / Poster: 120
Poster
Themen: Native MS
Stichworte: Native MS, Ebola virus, nucleoprotein, self-assembly

Analyzing self-assembly of Ebola virus nucleoprotein with native mass spectrometry

Janine Kopicki[1], Johannes Heidemann[1], Cesar Muñoz-Fontela[1], Charlotte Uetrecht[1,2]
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Poster-120-55.pdf

ID: 10 / Poster: 121
Poster
Themen: Native MS
Stichworte: Native mass spectrometry, human noroviruses, glycan-mimetics, P domain, binding interactions.

Native mass spectrometry analysis of norovirus - glycan mimetics interaction

Hao Yan[1], Katharina Bücher[2], Laura Hartmann[2], Robert Creutznacher[3], Alvaro Mallagaray[3], Thomas Peters[3], Charlotte Uetrecht[1,4]
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Poster-121-10.pdf

ID: 93 / Poster: 122
Poster
Themen: Native MS
Stichworte: Membrane Proteins, Native-MS, LILBID-MS, Top-Down-MS

From Salty to Salt-free: Monitoring the Salt-dependent Dissoziation of the Membrane Protein Complex GCD in a Single Experiment

Nils Hellwig[1], Stella Vitt[2], Ulrich Ermler[2], Nina Morgner[1]
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ID: 52 / Poster: 123
Poster
Themen: Native MS
Stichworte: Native mass spectrometry (MS), viral cell entry, glycan binding, structural changes

Studying viral capsid glycan interaction with native MS

Ronja Pogan[1], Julia Lockhauserbäumer[1], Hao Yan[1], Grant Hansman[2], Mario Schelhaas[3], Bärbel Blaum[4], Charlotte Uetrecht[1,5]
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Poster-123-52.pdf

ID: 202 / Poster: 124
Poster
Themen: Proteine & Proteomics, Lebensmittelanalytik
Stichworte: AGEs, aging, amino acid analysis, glycation, LC-MS

Profiles of glycated amino acid adducts in the protein hydrolyzates of pea (Pisum sativum) seeds subjected to accelerated ageing

Maria Vikhnina[1,2], Alena Soboleva[1,2], Tahir Mehmood[1], Ekaterina Romanovskaya[2], Galina Smolikova[3], Andrej Frolov[1], Sergei Medvedev[3]
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Poster-124-202.pdf

ID: 146 / Poster: 125
Poster
Themen: Proteine & Proteomics, Organische Massenspektrometrie
Stichworte: DNA-protein cross-links, RNPxl, diepoxybutane, TiO2 enrichment

Analysis of 1,2,3,4-diepoxybutane induced DNA-histone cross-links by mass spectrometry

Katharina Mucek[1], Alexandra Stützer[1], Aleksander Chernev[1], Henning Urlaub[1,2]
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Poster-125-146.pdf

ID: 73 / Poster: 126
Poster
Themen: Proteine & Proteomics, Organische Massenspektrometrie
Stichworte: human immunodeficiency virus, ID-MS, viral load

Precise quantification of HIV proteins by isotope dilution mass spectrometry (ID-MS) for applications in HIV diagnostics

Luise Luckau[1], André Henrion[1], Petra Mischnick[2], Bernd Güttler[1]
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Poster-126-73.pdf

ID: 195 / Poster: 127
Poster
Themen: Proteine & Proteomics, Sonstiges
Stichworte: On-plate digestion, On-plate reduction and alkylation, Oxidation, Method development, MALDI-MS

Investigating on-plate digestion of proteins with regard to trypsin activity and oxidation

Michael Rühl, Stefan Schönborn, Ute Bahr, Michael Karas
Goethe-Universität Frankfurt am Main, Deutschland; ruehl@pharmchem.uni-frankfurt.de

Poster-127-195.pdf

ID: 210 / Poster: 128
Poster
Themen: Proteine & Proteomics, Sonstiges
Stichworte: Neurological biomarkers identification

Applying a Proteoform profiling method for neurological disorder biomarker discovery operations

Ulrike Burmester[1], Jerome Vialaret[2], Sylvain Lehmann[2], Audrey Gabelle[2,3], Pierre-Olivier Schmit[4], Christophe Hirtz[2]
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ID: 204 / Poster: 129
Poster

Themen: Proteine & Proteomics
Stichworte: Galectin-3, affinity interaction, proteolytic extraction, mass spectrometry

CHARACTERIZATION OF CARBOHYDRATE BINDING SITES IN GALECTINS BY PROTEOLYTIC AFFINITY - MASS SPECTROMETRY

Yannick Baschung[1,2], Adrian Moise[3], Michael Przybylski[1]
[1]Steinbeis Centre Biopolymer Analysis & Biomedical Mass Spectrometry, Rüsselsheim, Germany; [2]Proteome Center, Institute of Immunology, University of Rostock, Rostock, Germany; [3]Department of Chemistry, University of Konstanz, Konstanz, Germany; yannick.baschung@hotmail.fr

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ID: 189 / Poster: 130
Poster
Themen: Proteine & Proteomics
Stichworte: Proteomics, Quantification, Label Free Quantification, Data Independent Acquisition

Comparison of label free quantification methods for proteomics

Dennis Krösser, Benjamin Dreyer, Pascal Steffen, Tobias Lange, Hartmut Schlüter
University Medical Center Hamburg-Eppendorf, Deutschland; d.kroesser@uke.de

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ID: 80 / Poster: 131
Poster
Themen: Proteine & Proteomics
Stichworte: Retinal guanylyl cyclase, cross-linking, GCAP, mass spectrometry

Structural Insights into Retinal Guanylyl Cyclase/GCAP-2 Interaction by Cross-linking and Mass Spectrometry

Anne Rehkamp, Tänzler Dirk, Christian Ihling, Andrea Sinz
Martin-Luther-University Halle-Wittenberg, Institute of Pharmacy, Department of Pharmaceutical Chemistry and Bioanalytics, Germany; anne.rehkamp@pharmazie.uni-halle.de

Poster-131-80.pdf

ID: 84 / Poster: 132
Poster
Themen: Proteine & Proteomics
Stichworte: Peptide Cross-Linking, (CID)-ESI-MS/MS, Protein structure analysis.

Synthesis of Isotope-Labeled Derivatives of the MS/MS-Cleavable Urea-Cross-Linker: Synthesis and Evaluation of Reactivity for Effective Protein Structure Analysis

Moritz Fischer[1], Christoph Hage[2], Mathias Schäfer[1], Andrea Sinz[2]
[1]Universität zu Köln, Deutschland; [2]Martin-Luther-Universität Halle-Wittenberg, Deutschland; mfisch11@smail.uni-koeln.de

Poster-132-84.pdf

ID: 98 / Poster: 133
Poster
Themen: Proteine & Proteomics
Stichworte: formate channel A, protein-interaction studies

Mass Spectrometry-Based Interaction Studies of the N-Terminus of the Formate Channel FocA from Escherichia coli

Jana Lorenz[1], Doreen Hunger[2], Gary Sawers[2], Andrea Sinz[1]
[1]Department of Pharmaceutical Chemistry and Bioanalytics, Institute of Pharmacy, Martin-Luther University Halle-Wittenberg, Halle (Saale), Germany; [2]Department of Microbiology, Institute of Biology, Martin-Luther University Halle-Wittenberg, Halle (Saale), Germany; jana.lorenz@pharmazie.uni-halle.de

Poster-133-98.pdf

ID: 215 / Poster: 134
Poster
Themen: Proteine & Proteomics
Stichworte: Beads, lysis, modification, extraction, preparation

A versatile method to extract, modify, enrich and digest proteomic samples directly from cell lysates

Yannik Lewin, Vahid Golghalyani, Michael Karas
Goethe Universität, Frankfurt, Deutschland; yannik.lewin@pharmchem.uni-frankfurt.de

Poster-134-215.pdf

ID: 175 / Poster: 135
Poster

Themen: Proteine & Proteomics
Stichworte: Quantitative Targeted Proteomics

Investigation of Q-TOF instruments advantages for label-free proteome analysis

Stephanie Kaspar-Schoenefeld, Markus Lubeck, Annette Michalski, Matthias Szesny, Pierre-Olivier Schmit
Bruker Daltonik GmbH, Deutschland; matthias.szesny@bruker.com

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ID: 62 / Poster: 136
Poster
Themen: Proteine & Proteomics
Stichworte: cross-linking, synaptic vesicles, protein complexes, protein interactions

Development of a protein interaction networks in synaptic vesicles using cross-linking and mass spectrometry

Sabine Wittig, Carla Schmidt
Interdisciplinary research center HALOmem, Martin Luther University Halle-Wittenberg, Kurt-Moses-Straße-3, 06120 Halle (Saale).; sabine.zurhorst@biochemtech.uni-halle.de

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ID: 91 / Poster: 137
Poster
Themen: Proteine & Proteomics
Stichworte: HDX-MS, PPARγ, phthalates, obesity

Phthalate metabolites MEHP and MEOHP but not the phthalate DEHP itself bind and activate the PPARγ

Isabel Kratochvil[1], Tommy Hofmann[1,2], Rita Schlichting[3], Beate Escher[3], Stefan Kalkhof[1,4], Martin von Bergen[1,5]
[1]Helmholtz-Centre for Environmental research (UFZ), Department of Molecular Systems Biology, Leipzig, Germany; [2]HALOmem, Halle (Saale), Germany; [3]Helmholtz-Centre for Environmental research (UFZ), Department of Cell Toxicology, Leipzig, Germany; [4]Coburg University, Department of Applied Sciences, Coburg, Germany; [5]University of Leipzig, Faculty of Biosciences, Pharmacy and Psychology, Leipzig, Germany; isabel.kratochvil@ufz.de

Poster-137-91.pdf

ID: 108 / Poster: 138
Poster
Themen: Proteine & Proteomics
Stichworte: T cell signaling, ADAP, Phosphorylation, Protein-Protein-Interaction

Analysis of serine-phosphorylation dependent protein-protein interactions of the T cell adaptor protein ADAP

Annika Manns[1], Michael Schümann[1], Heike Stephanowitz[1], Christian Freund[2], Eberhard Krause[1]
[1]Leibniz Institut für Molekulare Pharmakologie, Deutschland; [2]Institut für Chemie und Biochemie, Freie Universität Berlin, Deutschland; manns@fmp-berlin.de

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ID: 85 / Poster: 139
Poster
Themen: Proteine & Proteomics
Stichworte: 2D-LC, GelFree, high pH LC, Methanosarcina mazei, top-down

Combining 2D-LC-MS and Gelfree-LC-MS enhances both proteome coverage and the identification of short open reading frame encoded peptides

Liam Arron Cassidy[1], Daniela Prasse[2], Dennis Linke[1], Ruth A. Schmitz[2], Andreas Tholey[1]
[1]Div. Systematic Proteome Research & Bioanalytics, Institute for Experimental Medicine, Kiel University, Germany; [2]Institute for General Microbiology, Kiel University, Germany; l.cassidy@iem.uni-kiel.de

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ID: 245 / Poster: 140
Poster
Themen: Proteine & Proteomics
Stichworte: Differential centrifugation, SDS PAGE, in-gel digest, GeLC MS/MS analysis, label-free protein quantification

Improved protocol for recovery of vesicular proteins

Sofia Traikov, Nikolaj Zuleger, Henrik Thomas, Anna Shevchenko, Andrej Shevchenko
MPI of Cell Biology and Genetics, Dresden, Germany; traikov@mpi-cbg.de

Poster-140-245.pdf

ID: 113 / Poster: 141
Poster
Themen: Proteine & Proteomics
Stichworte: Quantitative Proteomics, 2D-LC MS, Isobaric Labeling, Alveolo-Capillary Barrier

Quantitative proteomics for the analysis of molecular changes in lung adenocarcinoma cells in response to Vitamin D3

Patrick Kaleja[1,2], Liam Cassidy[1], Sabine Fuchs[2], Andreas Tholey[1]
[1]AG Systematische Proteomforschung & Bioanalytik, Institut für Experimentelle Medizin, Christian-Albrechts-Universität, Kiel; [2]Klinik für Unfallchirurgie und Traumatologie, Experimentelle Unfallchirurgie, UKSH, Kiel; Kaleja.patrick@gmx.de

Poster-141-113.pdf

ID: 58 / Poster: 142
Poster
Themen: Proteine & Proteomics
Stichworte: SWATH, Micro Flow, Proteomics, Quantitation

Accelerating Data Independent Acquisition with Microflow Chromatography

Joerg Dojahn[1], Nick Morrice[2], Remco Van Soest[3], Christie Hunter[3]
[1]SCIEX, Deutschland; [2]SCIEX, UK; [3]SCIEX, USA; joerg.dojahn@sciex.com

Poster-142-58.pdf

ID: 220 / Poster: 143
Poster
Themen: Proteine & Proteomics
Stichworte: disulfide brigde reduction, biopharmaceuticals, antibodies, top-down MS

Evaluation of Optimal Conditions for Antibody Subunit Analysis on a Quadrupole-Orbitrap Mass Spectrometer

Kai Scheffler, Tabiwang Arrey, Martin Zeller, Eugen Damoc
Thermo Fisher Scientific, Deutschland; tabiwang.arrey@thermofisher.com

Poster-143-220.pdf

ID: 184 / Poster: 144
Poster
Themen: Proteine & Proteomics
Stichworte: Proteomics, Cold Stress, Plastids, Arabidopsis thaliana

Characterization of plastidal redox-responses during cold stress acclimation

Johannes Schütze, Hans-Peter Mock
IPK-Gatersleben, Deutschland; schuetzej@ipk-gatersleben.de

Poster-144-184.pdf

ID: 203 / Poster: 145
Poster
Themen: Proteine & Proteomics
Stichworte: Neo-glycoproteins, vaccine characterization, MALDI-MS, SPR

Innovative analytical methodologies for the development of new antitubercular agents

Francesca Rinaldi[1], Sara Tengattini[1], Caterina Temporini[1], Enrica Calleri[1], Gabriella Massolini[1], Loredana Lupu[2,3], Zdeněk Kukačka[2], Stefan Maeser[2], Michael Glocker[3], Michael Przybylski[2]
[1]Department of Drug Sciences, University of Pavia, Pavia, Italy; [2]Steinbeis Center for Biopolymer Analysis and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany; [3]Proteome Center, Institute of Immunology, University of Rostock, Rostock, Germany; francesca.rinaldi01@ateneopv.it

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ID: 135 / Poster: 146
Poster
Themen: Proteine & Proteomics
Stichworte: picosecond-infrared-laser, methionine oxidation, cancer, LC-MS/MS

Sampling of tissues with the picosecond-infrared-laser ablation for Redox Proteomics

Atef Mannaa[1], Marcel Kwiatkowski[1], Nils-Owe Hansen[2], R. J. Dwayne Miller[2], Hartmut Schlüter[1]
[1]Mass Spectrometric Proteomics, Department of Clinical Chemistry, University Medical Center Hamburg-Eppendorf, Hamburg, Germany.; [2]Max Planck Institute for the Structure and Dynamics of Matter, Atomically Resolved Dynamics Division, Luruper Chaussee 149, 22761 Hamburg, Germany.; atef.mannaa8@gmail.com

Poster-146-135.pdf

ID: 34 / **Poster: 147**
Poster
Themen: Proteine & Proteomics
Stichworte: post-translational modification, 2D gel electrophoresis, myelin, acetylome, tubulin acetylation

Partial Immunoblotting of 2D-Gels: A Novel Method to Identify Post-Translationally Modified Proteins Exemplified for the Myelin Acetylome

Kathrin Kusch[1], Marina Uecker[2], Thomas Liepold[2], Wiebke Möbius[1,3], Christian Hoffmann[4], Heinz Neumann[4], Hauke Werner[1], Olaf Jahn[2,3]

[1]Department of Neurogenetics, Max-Planck-Institute of Experimental Medicine, 37075 Göttingen, Germany; [2]Proteomics Group, Max-Planck-Institute of Experimental Medicine, 37075 Göttingen, Germany; [3]Center for Nanoscale Microscopy and Molecular Physiology of the Brain, 37075 Göttingen, Germany; [4]Free Floater (Junior) Research Group Applied Synthetic Biology, Georg-August University Göttingen, Institute for Microbiology and Genetics, 37077 Göttingen, Germany; jahn@em.mpg.de

Poster-147-34.pdf

50. Jahrestagung der Deutschen Gesellschaft für Massenspektrometrie

Datum: Dienstag, 07.03.2017

8:00 - 16:00	**Di_Tag: Tagungsbüro**
8:30 - 8:35 **Hörsaal 3**	**Di_Ank: Informationen**
8:35 - 9:20 **Hörsaal 3**	**Plenarvortrag 3: Massenspektrometrische Entwicklungen** Chair der Sitzung: **Jürgen Grotemeyer**

ID: 161 / **Plenarvortrag 3: 1**
Plenarvortrag
Stichworte: Plenary, Fundamentals

Adventures with Mass Spectrometers: From Designing New Catalysts to Developing a Non-Targeted Drug Metabolite Identification Procedure.

Richard A. J. O'Hair
The University of Melbourne, Australia; rohair@unimelb.edu.au

Plenarvortrag 3-1-161.pdf

9:20 - 10:05 **Hörsaal 3**	**Di_Pr: Mattauch-Herzog Förderpreis** Chair der Sitzung: **Michael Linscheid** Preisträger:Stephan Rauschenbach, Stuttgart
10:05 - 10:30	**Kaffeepause 4**
10:30 - 12:10 **Hörsaal 3**	**DiV_1a: Gasphasenreaktionen & Fragmentierungen II** Chair der Sitzung: **Dietmar Kuck**

10:30 - 10:50
ID: 20 / **DiV_1a: 1**
Vortrag
Themen: Gasphasenreaktionen & Fragmentierungen, Grundlagen der Massenspektrometrie
Stichworte: Fragmentierung, Fragmentierungsmechanismen, Anilinderivate, Isotopenmarkierung, Stoßaktivierung

Untersuchungen zu den unimolekularen und stoßaktivierten Fragmentierungsmechanismen der Diethyltoluidine über Isotopenmarkierungen

Sarah Seulen, Jürgen Grotemeyer
Christian-Albrechts-Universität zu Kiel, Deutschland; seulen@phc.uni-kiel.de

DiV_1a-1-20.pdf

10:50 - 11:10
ID: 173 / **DiV_1a: 2**
Vortrag
Themen: Gasphasenreaktionen & Fragmentierungen, Grundlagen der Massenspektrometrie
Stichworte: ETD, metallo-supramolecular-aggregates, one-electron reduction, self-assembly, gas phase reactivity

One-electron reduction of isolated metallo-supramolecular aggregates

Marianne Engeser
Universität Bonn, Deutschland; Marianne.Engeser@uni-bonn.de

DiV_1a-2-173.pdf

11:10 - 11:30
ID: 191 / **DiV_1a: 3**
Vortrag
Themen: Gasphasenreaktionen & Fragmentierungen
Stichworte: Formate attachment, ZnPorphyrin, ZnPhthalocyanine, true molecular dianions

Formate attachment to ZnPorphyrin- and ZnPhthalocyanine-Oligomers: Binding, Fragmentation, Affinity

Martin B. Minameyer[1], Jakob F. Hitzenberger[1], Stéphane Campidelli[2], Thomas Drewello[1]
[1]Friedrich-Alexander Universität Erlangen-Nürnberg, Deutschland; [2]LICSEN, NIMBE, CEA, CNRS, Université Paris-Saclay, France; martin.minameyer@fau.de

DiV_1a-3-191.pdf

11:30 - 11:50
ID: 37 / DiV_1a: 4
Vortrag
Themen: Gasphasenreaktionen & Fragmentierungen, Organische Massenspektrometrie
Stichworte: Triangulene, carbenium, OE vs. EE, energy-dependent CID

Reactivity and stability check of even vs. odd electron (quasi)-molecular ions derived from triangulenium type derivatives

Jakob F. Hitzenberger[1], Agnes Uhl[1], Ute Meinhardt[1], Pavlo O. Dral[2], Milan Kivala[1], Jürgen Schatz[1], Thomas Drewello[1]
[1]Friedrich-Alexander-University Erlangen-Nürnberg, Germany; [2]Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany; jakob.hitzenberger@fau.de

DiV_1a-4-37.pdf

11:50 - 12:10
ID: 97 / DiV_1a: 5
Vortrag
Themen: Gasphasenreaktionen & Fragmentierungen, Proteine & Proteomics
Stichworte: (-)-ESI-MS, peptide cross-linking, free radical-initiated peptide sequencing, TEMPO-Bz-linker, CID-cleavable cross-linker

Dissociation behavior of a TEMPO-benzyl cross-linker for peptide structure analysis by free radical initiated peptide sequencing (FRIPS) in negative ESI-MS

Christoph Hage[1], Mathias Schäfer[2], Andrea Sinz[1]
[1]Martin-Luther-Universität Halle-Wittenberg, Deutschland; [2]Universität zu Köln, Deutschland; christoph.hage@pharmazie.uni-halle.de

DiV_1a-5-97.pdf

10:30 - 12:10
Hörsaal 2

DiV_2a: Metabolomics

Chair der Sitzung: **Dietrich Volmer**

10:30 - 10:50
ID: 115 / DiV_2a: 1
Vortrag
Themen: Metaboliten & Metabolomics, Organische Massenspektrometrie
Stichworte: online-SPE-HILIC, Coenzym A Derivate, MS/MS

Online SPE-HILIC-ESI-MS/MS zur Untersuchung des Metabolismus von auf Acetyl-CoA und Malonyl-CoA in MCF-7 Brustkrebszellen

Alexander Schriewer, Heiko Hayen
WWU Münster, Deutschland; alexander.schriewer@wwu.de

DiV_2a-1-115.pdf

10:50 - 11:10
ID: 133 / DiV_2a: 2
Vortrag
Themen: Metaboliten & Metabolomics
Stichworte: metabolomics, LC/MS library

LC/MS²-standards library using high-resolution accurate mass (HRAM) platform for metabolomics research

Julica Folberth, Alaa Othman
University of Lübeck, Germany; julica.folberth@pharma.uni-luebeck.de

DiV_2a-2-133.pdf

11:10 - 11:30
ID: 132 / DiV_2a: 3
Vortrag
Themen: Klinische Diagnostik & Forensik, Metaboliten & Metabolomics
Stichworte: Vitamin D, Derivatisierung, ionische Flüssigkeiten, Zellsystem-Messung, HPLC-MS/MS

Direct aqueous measurement of 25-hydroxyvitamin D in cellular environments by LC-MS/MS using the novel chemical derivatization reagent MDBP

Miriam J. Müller[1], Heiko Bruns[2], Dietrich A. Volmer[1]
[1]Saarland University, Deutschland; [2]University Hospital Erlangen, Deutschland; miriam.mueller@uni-saarland.de

DiV_2a-3-132.pdf

11:30 - 11:50
ID: 227 / DiV_2a: 4
Vortrag

Themen: Metaboliten & Metabolomics, Lebensmittelanalytik
Stichworte: Fusarium graminearum, wheat stem base, plants, mass spectrometry imaging, metabolites

Imaging metabolites in wheat stem base-Fusarium graminearum interactions using high-resolution atmospheric pressure scanning microprobe MALDI mass spectrometry imaging (SMALDI-MSI)

Dhaka Ram Bhandari[1], Qing Wang[2], Bin Li[3], Andreas Römpp[4], Sven Gottwald[2], Bernhard Spengler[1]
[1]Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, Heinrich-Buff-Ring 17, 35392 Giessen, Germany; [2]Department of Plant Breeding, Justus Liebig University Giessen, Heinrich-Buff-Ring 26–32, 35392 Giessen, Germany; [3]Department of Chemistry, University of Illinois, 405 North Mathews Avenue, 61801 Urbana, Illinois, USA; [4]Department of Food Analysis, University of Bayreuth, E.-C.-Baumann-Str. 20, 95326 Kulmbach, Bayreuth, Germany;
Dhaka.R.Bhandari@anorg.Chemie.uni-giessen.de

DiV_2a-4-227.pdf

11:50 - 12:10
ID: 152 / DiV_2a: 5
Vortrag
Themen: Metaboliten & Metabolomics
Stichworte: HR-ESI-MS, Electrochemistry, Metabolism, Automation

Automated electrochemistry/mass spectrometry for high-throughput analysis of xenobiotics

Simon Gereon Scheeren, Uwe Karst
Westfälische Wilhelms-Universität Münster, Deutschland; simon.scheeren@uni-muenster.de

DiV_2a-5-152.pdf

10:30 - 12:10
Hörsaal 1

DiV_3a: Analytische Anwendungen II

Chair der Sitzung: **Wolfgang Schrader**

10:30 - 10:50
ID: 149 / DiV_3a: 1
Vortrag
Themen: Glyco-Analytik & Glycomics, Proteine & Proteomics
Stichworte: advanced glycation end products (AGEs), GC-MS, glycation, LC-MS, model peptides, plant biochemistry

Probing plant Maillard reaction by mass spectrometry in model peptide systems

Andrej Frolov[1,2], Nikita Schilyaev[3], Funmilayo Fagbadebo[1], Uta M. Herfurth[2], Elena Lukasheva[3], Tatiana Grishina[3], Claudia Birkemeyer[2], Gerd U. Balcke[4], Tatiana Bilova[1,2], Ludger A. Wessjohann[1]
[1]Leibniz-Institut für Pflanzenbiochemie, Abteilung Natur- und Wirkstoffchemie, Germany; [2]Universität Leipzig, Fakultät für Chemie und Mineralogie, Germany; [3]Universität St. Petersburg, Lehrstuhl Biochemie, Russia; [4]Leibniz-Institut für Pflanzenbiochemie, Stoffwechsel- und Zellbiologie, Germany;
afrolov@ipb-halle.de

DiV_3a-1-149.pdf

10:50 - 11:10
ID: 90 / DiV_3a: 2
Vortrag
Themen: Lipide & Lipidomics
Stichworte: Shotgun lipidomics, high resolution, FT MS, spectra processing

Intensity Independent Filtering of FT MS and FT MS/MS Spectra for Shotgun Lipidomics

Kai Schuhmann, Henrik Thomas, Andrej Shevchenko
Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Deutschland;
schuhman@mpi-cbg.de

11:10 - 11:30
ID: 192 / DiV_3a: 3
Vortrag
Themen: Glyco-Analytik & Glycomics, Proteine & Proteomics
Stichworte: Mass spectrometry, Etanercept, Glycosylation, Isoelectric focusing, Peptide mapping

Mass spectrometry evaluation of the Etanercept physicochemical properties

Ramin Fazel[1,2], Hartmut Schlüter[2]
[1]The University of Tehran, Iran; [2]Universitätsklinikum Hamburg-Eppendorf, Germany;
rmn.fzl@gmail.com

11:30 - 11:50
ID: 207 / DiV_3a: 4
Vortrag
Themen: MS - Informatik / Bioinformatik, Proteine & Proteomics
Stichworte: α-dicarbonyls, AGEs, aging, Arabidopsis thaliana, mass spectrometry, oxidative stress, protein glycation, proteomics

Age-related glycation hotspots in plant proteome

Tatiana Bilova[1,2,3], Gagan Paudel[1,2], Dominic Brauch[2,4], Svetlana Milrud[3,5], Rico Schmidt[6], Elena Tarakhovskaya[3], Nikita Shilyaev[5], Galina Smolikova[3], Alain Tissier[7], Thomas Vogt[7], Claudia Birkemeyer[2], Wolfgang Brandt[1], Andrea Sinz[6], Ludger A. Wessjohann[1], Andrej Frolov[1,2]
[1]Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry (Halle/Saale); [2]Faculty of Chemistry and Mineralogy, Universität Leipzig; [3]Department of Plant Physiology and Biochemistry, St. Petersburg State University, Russia; [4]Leibniz Institute of Plant Genetics and Crop Plant Research (Stadt Seeland); [5]Department of Biochemistry, St. Petersburg State University, Russia; [6]Institute of Pharmacy, Martin-Luther Universität Halle-Wittenberg; [7]Department of Cell and Metabolic Biology, Leibniz Institute of Plant Biochemistry (Halle/Saale); bilova.tatiana@gmail.com

DiV_3a-4-207.pdf

11:50 - 12:10
ID: 219 / DiV_3a: 5
Vortrag
Themen: Proteine & Proteomics, Sonstiges
Stichworte: UV-induced cross-linking, protein-DNA cross-links, chromatin, histones

Analysis of UV-induced DNA–protein cross-links in a chromatin model

Alexandra Stützer[1], Christin Kappert[1], Aleksandar Chernev[1], Katharina Kramer[2], Wolfgang Fischle[1,3], Henning Urlaub[1,4]
[1]Max Planck Institute for Biophysical Chemistry, Göttingen, Germany; [2]Max Planck Institute for Plant Breeding Research, Köln, Germany; [3]KAUST, Saudi Arabia; [4]University Medical Center Göttingen, Germany; alexandra.stuetzer@mpibpc.mpg.de

10:30 - 12:10
Hörsaal 4

DiV_4a: Ionen Mobilität

Chair der Sitzung: **Andreas Tholey**

10:30 - 10:50
ID: 235 / DiV_4a: 1
Vortrag
Themen: Instrumentelle Entwicklungen, Ionenmobilität
Stichworte: Ionenmobilität, Kollisionsquerschnitt, Massenspektrometrie, Driftzeit, Standardisierung

Standardised Collision Cross Section Measurements by Single Static Drift Field Ion Mobility Instrument in an Interlaboratory Study

Tim Causon[1], Rebecca Konietzny[2], Teresa Mairinger[1], Stephan Hann[1], Jody May[3], Sarah Stow[3], John McLean[3], Erin Baker[4], Xueyun Zheng[4], Ruwan Kurulugama[5], Alex Mordehai[5], Emma Rennie[5], George Stafford[5], Ed Darland[5], John Fjeldsted[5]
[1]BOKU Wien, Österreich; [2]Agilent Technologies, Waldbronn, Deutschland; [3]Vanderbilt University, USA; [4]Pacific Northwest National Laboratory, USA; [5]Agilent Technologies, Santa Clara, USA; tim.causon@boku.ac.at

DiV_4a-1-235.pdf

10:50 - 11:10
ID: 162 / DiV_4a: 2
Vortrag
Themen: Gasphasenreaktionen & Fragmentierungen, Ionenmobilität
Stichworte: Supramolecular Chemistry, Halogen Bonding, ESI-MS

Investigation of Dimeric and Hexameric Halogen-Bonded Supramolecular Capsules by ESI-MS and IM-MS

Ulrike Warzok[1], Lotta Turunen[2], Waldemar Hoffmann[1,3], Kevin Pagel[1,3], Kari Rissanen[2], Christoph A. Schalley[1]
[1]Freie Universität Berlin; [2]Department of Chemistry, NanoScience Center, University of Jyvaskyla, Finnland; [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin; ulrike.warzok@fu-berlin.de

DiV_4a-2-162.pdf

11:10 - 11:30
ID: 170 / DiV_4a: 3
Vortrag
Themen: Ionenmobilität, Native MS
Stichworte: Protein-protein interaction, epitope mapping, ESI-MS, gas-phase dissociation, ion mobility MS

Intact Transition Epitope Mapping - A mass spectrometric method for accurate, facile, and rapid identification of specific antibody-peptide reactivities

Michael O. Glocker[1], Yelena Yefremova[1], Bright D. Danquah[1], Kwabena F.M. Opuni[1], Hans-Jürgen Thiesen[2]
[1]Proteome Center Rostock, Deutschland; [2]Institute of Immunology, University of Rostock, Germany; michael.glocker@uni-rostock.de

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11:30 - 11:50
ID: 223 / DiV_4a: 4
Vortrag
Themen: Ionenmobilität, Native MS
Stichworte: CID, CIU, gas-phase protein (un-) folding

Formation and Properties of a Compact Protein Unfolding Intermediate in the Gas-phase

Knut Kölbel[1], Frank Sobott[2]
[1]Universiteit Antwerpen, Belgien; [2]Universiteit Antwerpen, Belgien; knut.koelbel@uantwerpen.be

DiV_4a-4-223.pdf

11:50 - 12:10
ID: 40 / DiV_4a: 5
Vortrag
Themen: Ionenmobilität, Glyco-Analytik & Glycomics
Stichworte: Chondroitin Sulfate, Disaccharide, Ion Mobility Spectrometry-Mass Spectrometry, NMR, Apparent Self-Diffusion Coefficient

Differentiation and relative quantification of chondroitin sulfate isomers by ion mobility spectrometry-mass spectrometry and pulsed-field gradient NMR

Katharina Lemmnitzer[1], Thomas Riemer[1], Michael Groessl[2], Rosmarie Süß[1], Richard Knochenmuss[2], Jürgen Schiller[1]
[1]University of Leipzig, Medical Faculty, Institute of Medical Physics and Biophysics; [2]Tofwerk, Uttigenstrasse 22, CH-3600 Thun, Switzerland; katharina.lemmnitzer@medizin.uni-leipzig.de

DiV_4a-5-40.pdf

12:15 - 14:00 **Seminarraum 26**	**Lunch 4: Lunchseminar Sciex** Spezielle Registrierung bei der Firma
12:15 - 14:00 **Hörsaal 4**	**Lunch 5: Lunchseminar Agilent** Spezielle Registrierung bei der Firma
12:15 - 14:00 **Seminarraum 30**	**Lunch 6: Lunchseminar Bruker** Spezielle Registrierung bei der Firma
14:00 - 15:00 **Hörsaal 3**	**DiN_1a: MS-Informatik/Bioinformatik** Chair der Sitzung: **Thomas Drewello**

14:00 - 14:20
ID: 208 / DiN_1a: 1
Vortrag
Themen: MS - Informatik / Bioinformatik, Proteine & Proteomics
Stichworte: Peptide Mapping, Protein Inference, Bioinformatics, Sequence Tags

PeptideMapper: Efficient and Versatile Amino Acid Sequence and Tag Mapping

Dominik Kopczynski[1], Marc Vaudel[2,3], Robert Ahrends[1]
[1]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Otto-Hahn-Str. 6b, 44227 Dortmund, Germany; [2]KG Jebsen Center for Diabetes Research, Department of Clinical Science, University of Bergen, Norway; [3]Center for Medical Genetics and Molecular Medicine, Haukeland University Hospital, Bergen, Norway; dominik.kopczynski@isas.de

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14:20 - 14:40
ID: 224 / DiN_1a: 2
Vortrag
Themen: MS - Informatik / Bioinformatik, Proteine & Proteomics
Stichworte: DIA, LFQ, DDA

Comparison of Data-Independent Acquisition (DIA) and Data-Dependent Acquisition (DDA) for label-free Quantification

Pascal Steffen, Hartmut Schlüter
University Medical Center Hamburg-Eppendorf, Deutschland; p.steffen@uke.de

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14:40 - 15:00
ID: 145 / DiN_1a: 3
Vortrag
Themen: MS - Informatik / Bioinformatik, Metaboliten & Metabolomics
Stichworte: food authentication/food fraud, metabolomic fingerprinting/profiling, UPLC-TW-IMS-HR-Q-ToF MS, organic/conventional food, tomatoes

Differentiation of organic and conventional farming of tomatoes by non-targeted metabolomic profiling using travelling-wave ion mobility high resolution mass spectrometry

Jens Luetjohann, Anna Bauer, Juergen Kuballa
GALAB Laboratories GmbH, Deutschland; luetjohann@galab.de

DiN_1a-3-145.pdf

14:00 - 15:00
Hörsaal 2

DiN_2a: Metabolomics

Chair der Sitzung: **Dietrich Volmer**

14:00 - 14:20
ID: 154 / DiN_2a: 1
Vortrag
Themen: Metaboliten & Metabolomics, Proteine & Proteomics
Stichworte: non-targeted metabolomics, proteomics, pathway mapping

Increasing arginine production in C. glutamicum by rational strain design using a combination of metabolomics and proteomics

Matthias Szesny
Bruker Daltonik GmbH, Deutschland; matthias.szesny@bruker.com

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14:20 - 14:40
ID: 121 / DiN_2a: 2
Poster
Themen: Metaboliten & Metabolomics
Stichworte: LESA-HRMS, microbial co-cultures, rhizosphere

Application of high-throughput MS screening to disentangle the bacterial metabolome

Riya Christina Menezes[1], Paolina Garbeva[2], Purva Kulkarni[1,3], Aleš Svatoš[1]
[1]Max Planck Institute for Chemical Ecology, Jena, Germany; [2]Department of Microbial Ecology, Netherlands Institute of Ecology, Wageningen, The Netherlands; [3]Lehrstuhl für Bioinformatik, Friedrich Schiller University, Jena, Germany; rmenezes@ice.mpg.de

DiN_2a-2-121.pdf

14:40 - 15:00
ID: 181 / DiN_2a: 3
Vortrag
Themen: Instrumentelle Entwicklungen
Stichworte: QTOF, ion mobility, CCS, isomers, lipids, flavonoids

The Next Generation Ion Mobility Separation (IMS) Adds A New Dimension to Substance Characterization and Identification

Detlev Suckau
Bruker Daltonik GmbH, Deutschland; detlev.suckau@bruker.com

DiN_2a-3-181.pdf

14:00 - 15:00
Hörsaal 1

DiN_3a: Lipide II

Chair der Sitzung: **Dominik Schwudke**

14:00 - 14:20
ID: 182 / DiN_3a: 1
Vortrag
Themen: Lipide & Lipidomics
Stichworte: MALDI-TOF MS; HPTLC; Cardiolipin; Cytochrome c; Free radicals.

Cytochrome c-mediated modification of cardiolipin

Uladzimir Barayeu[1], Jörg Flemmig[1], Oleg Shadyro[2], Jürgen Arnhold[1]
[1]University of Leipzig, Medical Faculty, Institute of Medical Physics and Biophysics, Härtelstrasse 16-18, 04107 Leipzig, Germany; [2]Belarusian State University, Department of Chemistry, Leningradskaya 14, 220006, Minsk, Belarus; Uladzimir.Barayeu@medizin.uni-leipzig.de

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14:20 - 14:40
ID: 193 / DiN_3a: 2
Vortrag

Themen: Lipide & Lipidomics
Stichworte: Lipidomics, software, LC-MS/MS, spectral library

A new bridge between targeted and non-targeted LC-MS/MS lipidomics

Bing Peng, Dominik Kopczynski, Robert Ahrends
Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Germany; bing.peng@isas.de

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14:40 - 15:00
ID: 164 / DiN_3a: 3
Vortrag
Themen: Lipide & Lipidomics
Stichworte: Lung tissue, emphysema, lipidomics, histopathology, multivariate statistics

Lipidomes of human lung tissues show distinct lipid metabolic alterations for lung cancer and pulmonary emphysema

Lars Florian Eggers[1], Julia Müller[2], Chakravarthy Marella[1], Verena Scholz[1], Henrik Watz[3,5], Christian Kugler[4], Klaus F. Rabe[4,5], Torsten Goldmann[2,5], Dominik Schwudke[1,5]
[1]Research Center Borstel, Division of Bioanalytical Chemistry, Parkallee 1-40, D-23845 Borstel, Germany.; [2]Pathology of the University Hospital of Lübeck and the Research Center Borstel, Clinical and Experimental Pathology, 23538 Lübeck and 23845 Borstel, Germany.; [3]Pulmonary Research Institute at LungenClinic Großhansdorf, Wöhrendamm 80, 22927 Großhansdorf.; [4]LungenClinic Großhansdorf, Wöhrendamm 80, 22927 Großhansdorf.; [5]Airway Research Center North, German Center for Lung Research, Wöhrendamm 80, 22927 Großhansdorf, Germany; leggers@fz-borstel.de

DiN_3a-3-164.pdf

15:00 - 15:45
Hörsaal 3

Plenarvortrag 4: „Ja wo seid Ihr denn alle? Von der (seriösen) Suche nach extraterrestrischem Leben“
Chair der Sitzung: **Jürgen Grotemeyer**

ID: 251 / Plenarvortrag 4: 1
Plenarvortrag
Stichworte: Exoplanets, Extraterrestrial life

Where are ye all? – On the (serious) search for extraterrestrial life

Wolfgang J. Duschl
Christian-Albrechts-Universität zu Kiel, Deutschland; wjd@astrophysik.uni-kiel.de

15:45 - 16:30
Hörsaal 3

DGMS: DGMS Miitgliederversammlung

16:30 - 18:30

Poster Session Dienstag Nachmittag
Autoren der Poster mit grader Posternummer sind anwesend.

ID: 244 / Poster: 1
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Grundlagen der Massenspektrometrie
Stichworte: McLafferty reaction, Substituent effects, Distonic ions, Hydrogen transfer, Proton affinity

2-Benzylindane radical cations in the gas phase (I): Substituent effects on a stereoselective McLafferty reaction and related hydrogen transfer processes

Hans-Friedrich Grützmacher, Dietmar Kuck
Department of Chemistry, Bielefeld University; dietmar.kuck@uni-bielefeld.de

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ID: 246 / Poster: 2
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Grundlagen der Massenspektrometrie
Stichworte: Hydrogen scrambling, McLafferty reaction, Substituent effects, Lifetime of ions, stereoselectivity

2-Benzylindane radical cations in the gas phase (II): Substituenteffects on regio- and stereoselective progressive hydrogen scramblingoccurring prior to unimolecular fragmentation

Dietmar Kuck, Hans-Friedrich Grützmacher
Department of Chemistry, Bielefeld University; dietmar.kuck@uni-bielefeld.de

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ID: 19 / Poster: 3
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Organische Massenspektrometrie
Stichworte: REMPI, Flugzeitmassenspektrometrie, Cluster

REMPI-Spektroskopie von nicht-kovalenten Anisol-Clustern

Thorben Reinert, Jürgen Grotemeyer
Christian-Albrechts-Universität zu Kiel, Deutschland; reinert@phc.uni-kiel.de

Poster-3-19.pdf

ID: 22 / **Poster: 4**
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Instrumentelle Entwicklungen
Stichworte: mass spectrometry, fullerenes, instrumentation, single particle analysis

Resolution enhancement by delayed ion extraction in a single-particle aerosol mass spectrometer

Christof Barth, Klaus Peter Hinz, Bernhard Spengler
Justus-Liebig Universität Giessen, Deutschland; christof.barth@chemie.uni-giessen.de

Poster-4-22.pdf

ID: 26 / **Poster: 5**
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Ionisationsmethoden
Stichworte: electrospray, phthalocyanine, crown ether, cluster, aggregate

Aggregation of a crown-ether decorated zinc-phthalocyanine by collision-induced desolvation providing insight into the electrospray mechanism

Ina Kellner[1], Uwe Hahn[2,3], Maximilian Dürr[1], Tomás Torres[2,4], Ivana Ivanović-Burmacović[1], Thomas Drewello[1]
[1]Friedrich-Alexander-University Erlangen-Nürnberg, Deutschland; [2]Universidad Autónoma de Madrid, Spain; [3]University of Strasbourg and CNRS, European School for Chemistry, Polymers and Materials (ECPM), France; [4]Instituto Madrileño de Estudios Avanzados (IMDEA)-Nanociencia, Spain; ina.kellner@fau.de

Poster-5-26.pdf

ID: 42 / **Poster: 6**
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Sonstiges
Stichworte: ESI Mass Spectrometry, Gas-Phase Reactivity, Reaction Intermediates, Kinetics, Reaction Mechanism

Direct Observation and Reactivity Studies of Organoferrates by Electrospray Ionization Mass Spectrometry

Tobias Parchomyk, Konrad Koszinowski
Georg-August-Universität Göttingen, Deutschland; tobias.parchomyk@chemie.uni-goettingen.de

Poster-6-42.pdf

ID: 33 / **Poster: 7**
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Proteine & Proteomics
Stichworte: Proteomics, Top-Down, Intact Protein, Electrospray Ionization, Collision-Induced Dissociation

Improving the sequence coverage in top-down MS/MS of proteins

Alexander Becker, Mohamed Mokhtar, Andreas Tholey
Christian-Albrechts-Universität zu Kiel, Deutschland; a.becker@iem.uni-kiel.de

Poster-7-33.pdf

ID: 95 / **Poster: 8**
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Organische Massenspektrometrie
Stichworte: Organometallic reagents – ESI mass spectrometry – gas phase reactivity – homogenous catalysis – cross-coupling

Constitution and gas phase reactivity of organocobaltates

Friedrich Kreyenschmidt, Konrad Koszinowski
Georg-August-Universität Göttingen, Institut für Organische und Biomolekulare Chemie; fkreyen@gwdg.de

Poster-8-95.pdf

ID: 5 / **Poster: 9**
Poster
Themen: Grundlagen der Massenspektrometrie, Instrumentelle Entwicklungen
Stichworte: Instrumentation, tandem mass spectrometry, UVPD, charge dependence, nESI

Implementation of Ultraviolet Photodissociation on a LTQ FT Ultra Mass Spectrometer and first Applications

Simon Becher, Mario Kompauer, Bernhard Spengler, Sven Heiles

Institut für Anorganische und Analytische Chemie; Justus-Liebig-Universität Gießen; Sven.Heiles@anorg.chemie.uni-giessen.de

Poster-9-5.pdf

ID: 169 / Poster: 10
Poster
Themen: Grundlagen der Massenspektrometrie, Ionisationsmethoden
Stichworte: MALDI plume, wavelength dependence, laser fluence, thermometer molecules, internal energies

The internal energy in a MALDI plume probed with thermometer molecules: Effects of laser excitation wavelength and laser fluence

Alexander Potthoff[1], Jens Soltwisch[1,2], Annika Koch[1], Klaus Dreisewerd[1,2]
[1]Institute for Hygiene, University of Münster, Robert-Koch-Str. 41, 48149 Münster, Germany; [2]Interdisciplinary Center for Clinical Research (IZKF), University of Münster, Domagkstr. 3, 48149 Münster, Germany; alexpotthoff@uni-muenster.de

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ID: 47 / Poster: 11
Poster
Themen: Grundlagen der Massenspektrometrie
Stichworte: MALDI-MS Imaging, MALDI matrix, Laser wavelength, Absorption profile, Ion yield

Colorful MALDI: Effect of the Laser Excitation Wavelength on the Analytical Sensitivity in Standard MALDI-MS and Imaging Experiments

Annika Koch[1], Jens Soltwisch[1], Klaus Dreisewerd[1,2]
[1]University of Münster, Institute of Hygiene, Biomedical Mass Spectrometry, Germany; [2]Interdisciplinary Center for Clinical Research (IZKF) Münster, Germany; annika.koch@uni-muenster.de

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ID: 14 / Poster: 12
Poster
Themen: Grundlagen der Massenspektrometrie, Ionisationsmethoden
Stichworte: Atmosphärenbedingungen, Cluster, LTP, Twin-Trap, Cassini-Falle

Untersuchung von Limonen-Clustern im LTP-Twin-Trap Massenspektrometer

Björn Raupers[1], Claus Köster[2], Jürgen Grotemeyer[1]
[1]Universität Kiel, Deutschland; [2]Bruker-Daltonik GmbH, Bremen; raupers@phc.uni-kiel.de

Poster-12-14.pdf

ID: 103 / Poster: 13
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Grundlagen der Massenspektrometrie
Stichworte: thermometer ions, dissociation energy, kinetic shift, SSACM

An improved approach for calculating dissociation rates of benzylpyridinium ions

Thomas Auth, Konrad Koszinowski
Institut für Organische und Biomolekuare Chemie, Georg-August-Universität Göttingen, Deutschland; thomas.auth@chemie.uni-goettingen.de

Poster-13-103.pdf

ID: 70 / Poster: 14
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Organische Massenspektrometrie
Stichworte: ESI-MS, gas-phase chemistry, palladium-catalyzed cross-coupling, catalyst activation

Stability and Unimolecular Reactivity of Organopalladate(II) Complexes

Marlene Kolter, Konrad Koszinowski
Georg-August-Universität Göttingen, Deutschland; marlene.kolter@chemie.uni-goettingen.de

Poster-14-70.pdf

ID: 48 / Poster: 15
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Organische Massenspektrometrie
Stichworte: coinage metals, ate-complexes, organometallic compounds, reactive intermediates

Coinage-Metal Ate Complexes – An ESI-MS Study

Sebastian Weske[1], Richard O'Hair[2], Konrad Koszinowski[1]
[1]Georg-August-University Göttingen, Germany; [2]University of Melbourne, Australia; sebastian.weske@chemie.uni-goettingen.de

Poster-15-48.pdf

ID: 123 / **Poster: 16**
Poster
Themen: Gasphasenreaktionen & Fragmentierungen
Stichworte: ETD, metallo-supramolecular-aggregates, one-electron reduction, self-assembly, gas phase reactivity

ETD experiments on self-assembled asymmetric supramolecular squares

Yvonne Lorenz, Marianne Engeser
Universität Bonn, Deutschland; ylorenz@uni-bonn.de

Poster-16-123.pdf

ID: 86 / **Poster: 17**
Poster
Themen: Gasphasenreaktionen & Fragmentierungen
Stichworte: Ag+ adducts, helicene, π-π stacking, Energy-dependent CID

Formation and structure elucidation of $[M_2$ and $Ag]^+$ ions with M = [6]helicene, [7]helicene and coronene

Vera Warmbrunn, Martin Minameyer, Thomas Drewello
Friedrich-Alexander-University Erlangen-Nürnberg, Germany; vera.warmbrunn@fau.de

Poster-17-86.pdf

ID: 88 / **Poster: 18**
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Grundlagen der Massenspektrometrie
Stichworte: Crystallization, fragmentation behavior, slow heating CID, resonant ion excitation, quadrupole ion trap

Formation and dissociation behavior of multiply charged salt-like cluster ions (sodium formate)

Thomas Neugebauer, Thomas Drewello
Friedrich-Alexander-University Erlangen-Nürnberg, Deutschland; thomas.neugebauer@fau.de

Poster-18-88.pdf

ID: 65 / **Poster: 19**
Poster
Themen: Gasphasenreaktionen & Fragmentierungen, Grundlagen der Massenspektrometrie
Stichworte: Photodissoziation, CID, FT-ICR, Laserfarbstoffe

Wellenlängenabhängige Photofragmentierung von fluoreszierenden Farbstoffen in einem FT-ICR Massenspektrometer

Elena Mitrofanov, Tassilo Muskat, Jürgen Grotemeyer
Christian-Albrechts-Universität, Deutschland; mitrofanov@phc.uni-kiel.de

Poster-19-65.pdf

ID: 39 / **Poster: 20**
Poster
Themen: Klinische Diagnostik & Forensik
Stichworte: New psychoactive substances; NPS; library; LC-MS/MS; QTrap;

Update of an MS/MS Library of NPS for QTRAP® instruments

Katharina Grafinger[1], Lars Ambach[1,2], Florian Franz[3], Verena Angerer[3], Wolgang Weinmann[1]
[1]Universtität Bern, Institut für Rechtsmedizin, Forensische Toxikologie und Chemie, Switzerland; [2]Universität Ghent, Department of Bioanalysis, Laboratory of Toxicology, Belgium; [3]Universitätsklinikum Freiburg, Institut für Rechtsmedizin, Forensische Toxikologie, Germany; katharina.grafinger@irm.unibe.ch

Poster-20-39.pdf

ID: 106 / **Poster: 21**
Poster
Themen: Klinische Diagnostik & Forensik
Stichworte: LC-MS, antibiotics, tuberculosis, therapeutic drug monitoring

LC-MS2 Method Development for Simultaneous Analysis of Antibiotics from Plasma of MDR-TB Patients

Hande Karaköse[1,3], Niklas Köhler[2,3], Christoph Lange[2,3,4], Patricia Sanchez-Carballo[2,3], Dominik Schwudke[1,3]
[1]Division of Bioanalytical Chemistry, Research Center Borstel, Germany; [2]Division of Clinical Infectious Diseases, Research Center Borstel, Borstel, Germany; [3]German Center for Infection

Research, Clinical Tuberculosis Center, Borstel, Germany; [4]International Health/Infectious Diseases, University of Lübeck, Lübeck, Germany; hkarakoese@fz-borstel.de

Poster-21-106.pdf

ID: 200 / Poster: 22
Poster
Themen: Ionisationsmethoden, Native MS
Stichworte: Atmosphärendruck Ionisation, Papierbasierte Massenspektrometrie, Mikrofluidik, Instrumentelle Entwicklung

Modifikation von Papiersubstraten mit hydrophoben Barrieren zur Erhöhung der Empfindlichkeit und Reproduzierbarkeit in der papierbasierten Massenspektrometrie

Yves U. Hachenberger[1], Knut Rurack[2], Michael W. Linscheid[1], Jens Riedel[2]
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Poster-22-200.pdf

ID: 160 / Poster: 23
Poster
Themen: Ionisationsmethoden, Organische Massenspektrometrie
Stichworte: Pyrolysis bio-oil, Ionization techniques, Composition analysis

Characterization of Fast-Pyrolysis Bio-Oil

Yun Xu, Wolfgang Schrader
Max-Planck-Institut für Kohlenforschung, Deutschland; yxu@kofo.mpg.de

Poster-23-160.pdf

ID: 77 / Poster: 24
Poster
Themen: Ionisationsmethoden, Umweltanalytik
Stichworte: Nano Particle Analysis, Extractive Electrospray Ionization, Online Analysis

Characterization of a New Extractive Electrospray Ionization (EESI) Source for Online Particle Analysis and its Application to Atmospheric Aerosol

Felipe Lopez-Hilfiker[1,2], Sonja Klee[1], Manuel Hutterli[1], Veronika Pospilova[2], Jay Slowik[2]
[1]TOFWERK, Schweiz; [2]Paul Scherrer Institute (PSI), Villigen, Switzerland; klee@tofwerk.com

Poster-24-77.pdf

ID: 30 / Poster: 25
Poster
Themen: Ionisationsmethoden, Native MS
Stichworte: native MS, softness of ionization, laser desorption, energy distributions, binding affinities

Characterizing the LILBID ionization method: energy transfer and dissociation

Phoebe Young, Isabell Grübner, Genia Hense, Nina Morgner
Goethe Universität Frankfurt, Deutschland; young@chemie.uni-frankfurt.de

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ID: 127 / Poster: 26
Poster
Themen: Element- & Speziationsanalytik, Organische Massenspektrometrie
Stichworte: liquid crystal display, sealant, laser ablation, APCI-MS, ICP-MS

Analysis of Liquid Crystal Display Sealants using Spatially Resolved Mass Spectrometric Methods

Jennifer-Christin Mueller[1], Claudia Enders[2], Peter Leonhard[2], Uwe Karst[1]
[1]Institute of Inorganic and Analytical Chemistry, University of Muenster, Corrensstr. 28/30, 48149 Muenster, Germany; [2]Merck KGaA, Frankfurter Str. 250, 64293 Darmstadt, Germany; jennifer.mueller@uni-muenster.de

Poster-26-127.pdf

ID: 143 / Poster: 27
Poster
Themen: Element- & Speziationsanalytik, Umweltanalytik
Stichworte: ICP-MS, nanoparticles, TOF

Determination of multi-element composition and mass of single nanoparticles in liquids and air

Urs Rohner, Patrick Sturm, Olga Borovinskaya, Martin Tanner
TOFWERK, Switzerland; rohner@tofwerk.com

ID: 144 / **Poster: 28**
Poster
Themen: Ionisationsmethoden, Klinische Diagnostik & Forensik
Stichworte: Laser ablation, high resolution mass spectrometry, drug analysis, synthetic cannabinoids

Molecular laser ablation-mass spectrometry for rapid identification of synthetic cannabinoids

Elias Lützen[1], Uwe Karst[1], Sascha Münster-Müller[2], Michael Pütz[2]
[1]Westfählische Wilhelms-Universität Münster; [2]Bundeskriminalamt Wiesbaden; eliasluetzen@uni-muenster.de

Poster-28-144.pdf

ID: 109 / **Poster: 29**
Poster
Themen: Klinische Diagnostik & Forensik, Proteine & Proteomics
Stichworte: pesticides, organophosphates, mass spectrometry, biomarkers, albumin adducts

Albumin adducts as biomarkers of an exposure with organophosphorus pesticides

Jens von der Wellen, Horst Thiermann, Harald John
Bundeswehr Institute of Pharmacology and Toxicology; jensvonderwellen@bundeswehr.org

Poster-29-109.pdf

ID: 247 / **Poster: 30**
Poster
Themen: Klinische Diagnostik & Forensik, Proteine & Proteomics
Stichworte: Rheumatoid arthritis, mass spectrometry, oxidative stress, post translational modification

Identification of oxidative biomarkers in synovial fluid of patients suffering from rheumatoid arthritis

Dennis Westphal[1], Maria Fedorova[1,2], Ralf Hoffmann[1,2]
[1]Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig, Germany; [2]Center for Biotechnology and Biomedicine, Universität Leipzig, Germany; dennis.westphal@bbz.uni-leipzig.de

Poster-30-247.pdf

ID: 110 / **Poster: 31**
Poster
Themen: Klinische Diagnostik & Forensik, Proteine & Proteomics
Stichworte: Sulfur mustard, N-acetylcysteine, high-resolution mass spectrometry, scavenger, albumin adducts

Mass spectrometric investigation of N acetylcysteine as a potential scavenger against sulfur mustard

Markus Siegert[1], Horst Thiermann[2], Harald John[2]
[1]Department of Chemistry, Humboldt Universität zu Berlin, Berlin, Germany; [2]Bundeswehr Institute of Pharmacology and Toxicology, Munich, Germany; markus.siegert@student.hu-berlin.de

Poster-31-110.pdf

ID: 59 / **Poster: 32**
Poster
Themen: Klinische Diagnostik & Forensik, Proteine & Proteomics
Stichworte: autoimmunity, biomarker identification, MALDI-TOF mass spectrometry, immunoprecipitation

The role of mass spectrometry in the identification of autoantigens as targets in neurological autoimmune diseases

Madeleine Scharf, Ramona Miske, Stephanie Kade, Stefanie Hahn, Nora Begemann, Yvonne Denno, Christian Probst, Bianca Teegen, Kathrin Borowski, Winfried Stöcker, Lars Komorowski
Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany; n.begemann@euroimmun.de

Poster-32-59.pdf

ID: 239 / **Poster: 33**
Poster
Themen: Klinische Diagnostik & Forensik, Proteine & Proteomics
Stichworte: Proteomics, Protein mass spectrometric analysis, Skin, database for epidermis and dermis

Proteomic investigation of skin cell layers by tissue ablation using picosecond infrared laser (PIRL)

Parnian Kiani[1], Hartmut Schlüter[1], Jörn Hendrik Reuter[2], Tanja Bussmann[2], Nils-Owe Hansen[3], Stephanie Uschold[3], R. J. Dwayne Miller[3], Dennis Eggert[4]
[1]University Medical Centre Hamburg-Eppendorf, Institute for Clinical Chemistry, Department for Mass Spectrometric Proteomics, Hamburg; [2]Research and Development, Beiersdorf AG, Hamburg; [3]Max Planck Institute for the Structure and Dynamics of Matter CFEL, Hamburg; [4]Heinrich Pette Institute, Leibniz Institute for Experimental Virology, Hamburg; pkiani@uke.de

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ID: 99 / Poster: 34
Poster
Themen: Klinische Diagnostik & Forensik, Metaboliten & Metabolomics
Stichworte: N-Acetyltaurine, Taurine, Alcohol marker, Abstinence monitoring, Urine analysis, LC-MS/MS

N-Acetyltaurine as a novel urinary ethanol marker in a drinking study

Marc Luginbühl[1], Sofie Rutjens[2], Stefan Koenig[1], Julien Furrer[3], Wolfgang Weinmann[1]
[1]Institute of Forensic Medicine, University of Bern; [2]Laboratory of Toxicology, University of Ghent; [3]Department of Chemistry and Biochemistry, University of Bern; marc.luginbuehl@irm.unibe.ch

Poster-34-99.pdf

ID: 214 / Poster: 35
Poster
Themen: Klinische Diagnostik & Forensik, Sonstiges
Stichworte: Explosives, HPLC, HR-MS

Differentiation and Identification of Explosives Formulations by Means of HPLC-MS

Tilo D. Schachel, Uwe Karst
Westfälische Wilhelms-Universität Münster, Deutschland; tilo.schachel@uni-muenster.de

Poster-35-214.pdf

ID: 212 / Poster: 36
Poster
Themen: Ionenmobilität, Klinische Diagnostik & Forensik
Stichworte: tetrahydrocannabinol, cannabidiol, marijuana, ion mobility-MS, forensic chemistry

Separation of isomeric cannabinoids by high-resolution ion mobility-MS for the differentiation of legal and illegal marijuana

Marianne Hädener[1], Wolfgang Weinmann[1], Michael Groessl[2]
[1]University of Bern, Institute of Forensic Medicine, Forensic Toxicology and Chemistry, Bühlstrasse 20, 3012 Bern, Switzerland; [2]TOFWERK, Uttigenstrasse 22, 3600 Thun, Switzerland; marianne.haedener@irm.unibe.ch

Poster-36-212.pdf

ID: 241 / Poster: 37
Poster
Themen: Instrumentelle Entwicklungen, Klinische Diagnostik & Forensik
Stichworte: DSA, TOF, LC, Screening

Rapid Screening of Methylamphetamine in Hair of Drug Addicts using DSA-TOF

Stefan Edler
LAS Perkinelmer GmbH, Deutschland; stefan.edler@perkinelmer.com

Poster-37-241.pdf

ID: 248 / Poster: 38
Poster
Themen: Instrumentelle Entwicklungen
Stichworte: mass spectrometry, instrumentation, single particle analysis, delayed ion extraction

Optimization of the LAMPAS 3 laser mass spectrometer for improved on-line single particle analysis

Klaus-Peter Hinz, Christof Barth, Bernhard Spengler
Justus-Liebig-Universität Gießen, Deutschland; Klaus-Peter.Hinz@anorg.Chemie.uni-giessen.de

Poster-38-248.pdf

ID: 131 / Poster: 39
Poster
Themen: Instrumentelle Entwicklungen
Stichworte: tandem mass spectrometry, time of flight, high resolving power, high separation power

Tandem Mass Spectrometry with a (Ultra-)High Resolving Time-of-Flight Mass Spectrometer

Julian Bergmann[1], Wayne Lippert[1], Johannes Lang[1], Timo Dickel[1,2], Wolfgang R. Plaß[1,2], Hans Geissel[1,2], Christoph Scheidenberger[1,2], Mikhail Yavor[3], Alexander Pikhtelev[4], Samuel Ayet San Andrés[1,2]

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Poster-39-131.pdf

ID: 83 / Poster: 40
Poster
Themen: Instrumentelle Entwicklungen
Stichworte: Field ionisation, FI, GCMS, molecular weight determination

Field ionization: an old but still useful method

Christian Bartelmus, Sophie Brogly, Oliver Scheidegger
Hoffmann la Roche AG, Schweiz; christian.bartelmus@roche.com

ID: 218 / Poster: 41
Poster
Themen: Instrumentelle Entwicklungen, Umweltanalytik
Stichworte: on site analysis, portable GC/MS

Rapid On Site Analysis of BTX with Portable GC/MS

Martin Dinse, Alan Gallaspy, Bill Hahn, Charlie Schmidt
PerkinElmer LAS (Germany) GmbH, Deutschland; martin.dinse@perkinelmer.com

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ID: 250 / Poster: 42
Poster
Themen: Instrumentelle Entwicklungen, Ionisationsmethoden
Stichworte: Single particle aerosol mass spectrometry, ATOFMS, laser desorption–laser post ionization, LDI polycyclic aromatic hydrocarbons, inorganic core

Multiple analysis of individual airborne aerosol particles by laser mass spectrometry: Detection of polyaromatic hydrocarbons from the particle-surface and particle-core

Johannes Passig[1], Julian Schade[1], M. Fuchs[2], M. Oster[2], Martin Sklorz[1], Ralf Zimmermann[1,2]
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Poster-42-250.pdf

ID: 124 / Poster: 43
Poster
Themen: Instrumentelle Entwicklungen
Stichworte: Photoionisation, Fuel Characterisation, Thermal Analysis

Thermogravimetry coupled to Ultrafast Gas Chromatography Singlephoton-Ionisation Time-of-Flight-Mass-Spectrometry (TG-SPI-TOF-MS) for Evolved-Gas-Analysis of Fuels regarding to the Deposit Formation Potential

Anne Ulbrich[1], Winfried Koch[2], Sebastian Wohlfahrt[3], Michael Fischer[3], Thorsten Streibel[1,3], David Diarra[2], Ralf Zimmermann[1,3]
[1]Universität Rostock, Deutschland; [2]Oil-Wärme-Institut GmbH, Herzogenrath, Deutschland; [3]Helmholtz-Zentrum München,Deutschland; anne.ulbrich@uni-rostock.de

Poster-43-124.pdf

ID: 179 / Poster: 44
Poster
Themen: Instrumentelle Entwicklungen, Ionisationsmethoden
Stichworte: Single-photon ionization, SALDI, elevated pressure ion source, oMALDI2, laser mass spectrometry

Single-photon ionization of laser desorbed molecules in a fine-vacuum ion source

Christoph H. M. Bookmeyer[1], Andreas Schnapp[1], Klaus Dreisewerd[1,2]
[1]Institute for Hygiene, University of Münster, Robert-Koch-Str. 41, 48149 Münster, Germany; [2]Interdisciplinary Center for Clinical Research (IZKF), University of Münster, Domagkstr. 3, 48149 Münster, Germany; c_book01@uni-muenster.de

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ID: 217 / Poster: 45
Poster
Themen: Instrumentelle Entwicklungen, Native MS
Stichworte: Antibodies, Biopharmaceuticals, Native MS, high mass range

Full Characterization of Antibodies Under Denaturing and Native Conditions on a Hybrid Quadrupole-Orbitrap MS Equipped With a Higher Mass Range

Kai Scheffler[1], Eugen Damoc[1], Tabiwang Arrey[1], Martin Zeller[1], Jennifer Sutton[2], Aaron Bailey[2], Jonathan Josephs[2]
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Poster-45-217.pdf

ID: 111 / Poster: 46
Poster
Themen: Instrumentelle Entwicklungen, Lipide & Lipidomics
Stichworte: Lipidomics, DIQ, new data independent acquisition method

Lipidomics Quantitation Using a Novel Scanning Quadrupole DIA Method

Gunnar Weibchen[1], Chris Hughes[2], Keith Richardson[2], Jason Wildgoose[2], Lee Gethings[2], James Langridge[2]
[1]Waters GmbH, Germany; [2]Waters Corporation, Wilmslow, United Kingdom;
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Poster-46-111.pdf

ID: 240 / Poster: 47
Poster
Themen: Instrumentelle Entwicklungen, Umweltanalytik
Stichworte: high resolution mass spectrometry, evolved gas analysis, atmospheric pressure ionisation, thermal desorption, laser desorption

Thermal and laser desorption atmospheric pressure photo ionisation ultra high resolution mass spectrometry – Concept and application towards complex samples

Anika Neumann[1], Christopher Rüger[1], Martin Sklorz[1], Ralf Zimmermann[1,2,3]
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anika.neumann2@uni-rostock.de

Poster-47-240.pdf

ID: 35 / Poster: 48
Poster
Themen: Instrumentelle Entwicklungen, Proteine & Proteomics
Stichworte: SONAR, Quantification, Proteomics, DIA, Scanning

Quantitation of Proteomics Samples Using a Novel Scanning Quadrupole DIA Method

Marc Kipping[1], Chris Hughes[2], Keith Richardson[2], Jason Wildgoose[2], Lee Gethings[2], James Langridge[2], John Hoyes[2], Johannes PC Vissers[2]
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ID: 46 / Poster: 49
Poster
Themen: Instrumentelle Entwicklungen, Ionisationsmethoden
Stichworte: Ambient mass spectrometry, Ionization, Emission spectroscopy, Laser induced plasma, High repetition rate laser

Improving the performance of the airborne laser-spark ion source for the detection of volatile organic compounds under ambient conditions

Andreas Bierstedt, Jens Riedel
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Poster-49-46.pdf

ID: 174 / Poster: 50
Poster
Themen: Instrumentelle Entwicklungen
Stichworte: trapped ion mobility ms

High resolution trapped ion mobility mass spectrometry analysis of isomeric compounds

Sven W. Meyer, Ulrike Burmester
Bruker Daltonik GmbH, Deutschland; ulrike.burmeater@bruker.com

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ID: 172 / Poster: 51
Poster
Themen: Instrumentelle Entwicklungen
Stichworte: Direct Inlet Probe, Time-of-flight MS, High Resolution MS

The Usage of Direct Inlet Probe in combination with High Resolution Mass Spectrometry

Juergen Wendt[1], Uwe Kaefer[2]
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ID: 66 / Poster: 52
Poster
Themen: Instrumentelle Entwicklungen, Ionenmobilität
Stichworte: IR-MALDI, ion mobility, structure, peptides, collision cross-sections

IR-MALDI Ion Mobility Spectrometry: Low and High Field Mobilities of Peptide Ions at Intermediate Pressure

José Villatoro[1,3,4], Daniel Riebe[1], Toralf Beitz[1], Marcus Weber[2], Hans-Gerd Löhmannsröben[1]
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Poster-52-66.pdf

ID: 56 / Poster: 53
Poster
Themen: Instrumentelle Entwicklungen, Native MS
Stichworte: LILBID QTOF, Native Mass Spectrometry, Protein net charge

Monitoring and correlating of protein charge states with respect to amino acid modification and buffer conditions

Kudratullah Karimi, Jan Hoffmann, Nils Hellwig, Nina Morgner
Goethe-University Frankfurt/Main, Deutschland; k_kudratullah@hotmail.de

Poster-53-56.pdf

ID: 45 / Poster: 54
Poster
Themen: Lipide & Lipidomics
Stichworte: UV-LDI-MS, lipids, double bond position, ozonolysis, MS/MS

Elucidation of double bond positions in lipids by means of off-line ozonolysis followed by ultraviolet laser desorption ionization mass spectrometry

Eike Ulrich Brockmann[1], Andreas Schnapp[1], Klaus Dreisewerd[1,2]
[1]Institute for Hygiene, Biomedical Mass Spectrometry, University of Münster, Germany; [2]Interdisciplinary Center for Clinical Research (IZKF), University of Münster, Germany; eike.brockmann@ukmuenster.de

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ID: 168 / Poster: 55
Poster
Themen: Lipide & Lipidomics
Stichworte: Lipidomics, Fatty acid metabolism, Proteomics

SIMPLEX reveals myoglobin as a key player in cardiac lipid metabolism

Cristina Coman[1], Ulrike B. Hendgen-Cotta[2], Sonja Esfeld[2], Robert Ahrends[1], Matthias Totzeck[2]
[1]Leibniz-Institut für Analytische Wissenschaften – ISAS e.V., Germany; [2]University Hospital Essen, Medical Faculty, West German Heart and Vascular Center, Department of Cardiology and Department of Angiology, Germany; cristina.coman@isas.de

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ID: 238 / Poster: 56
Poster
Themen: Lipide & Lipidomics
Stichworte: PIRL, DIVE, Lipids, DDA

Lipidomics of Pig Brain Using the PIRL-DIVE Homogenisation Technique

Marceline Manka Fuh[1], Marcus Wurlitzer[1], Dominik Schwudke[2], Nils-Owe Hansen[3], Dwayne Miller[3], Hartmut Schlüter[1]

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Poster-56-238.pdf

ID: 141 / Poster: 57
Poster
Themen: Lipide & Lipidomics
Stichworte: UPLC-MS/MS, diacyl-glycerophospholipids, negative ion ESI, structural isomer mixtures

Spotting of Structural Isomer Mixtures of Diacyl-Glycerophospholipids via UPLC-MS/MS

Wolf-Dieter Lehmann[1,2], Katharina Wozny[2], Britta Brügger[2]
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Poster-57-141.pdf

ID: 114 / Poster: 58
Poster
Themen: Lipide & Lipidomics
Stichworte: Brustkrebszellen, HILIC, Phospholipide, Lipidprofiling, BMP

Profiling von konfigurationsisomeren Phospholipiden mittels HILIC-ESI-MS/MS

Christian Vosse, Heiko Hayen
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Poster-58-114.pdf

ID: 50 / Poster: 59
Poster
Themen: Ionenmobilität, Lipide & Lipidomics
Stichworte: Detergens removal, Lipidomics, SelexIon

SelexION® DMS-based detergent interference removal for shotgun-lipidomics analyses

Cyrus Papan[1], Julian Langer[2]
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Poster-59-50.pdf

ID: 102 / Poster: 60
Poster
Themen: Lipide & Lipidomics
Stichworte: Lipidanalytik, Doppelbindungsposition, Paternò Büchi Reaktion

Bestimmung von Doppelbindungspositionen in Lipiden mittels photochemischer Nachsäulenderivatisierung und Tandem-MS

Viola Jeck, Heiko Hayen
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Poster-60-102.pdf

ID: 126 / Poster: 61
Poster
Themen: Lipide & Lipidomics
Stichworte: electrochemical oxidation, mass spectrometry detection, lipid oxidation

In situ monitoring of lipid oxidation using electrochemistry-mass spectrometry coupling

Giulia Coliva[1,2], Simone Colombo[3], Agnieszka Kraj[4], Jean-Pierre Chervet[4], M. Rosario Domingues[3], Pedro Domingues[3], Maria Fedorova[1,2]
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Poster-61-126.pdf

ID: 159 / Poster: 62
Poster
Themen: Metaboliten & Metabolomics
Stichworte: human endogenous metabolites

Enabling High-Confidence Human Endogenous Metabolite Identification via High-Resolution MS/MS Retention-Time Library

Nan Wang[1], Stephan Kühne[2], Aiko Barsch[2], Ulrike Schwaiger-Hufnagel[2], Xian Luo[1], Shuang Zhao[1], Yiman Wu[1], Zhendong Li[1], Wei Han[1], Jaspaul Tatlay[1], Yunong Li[1], Kevin Hooton[1], Dorothea Mung[1], Adriana Buzatto[1], Xiaohang Wang[1], Liang Li[1]

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ID: 157 / Poster: 63
Poster
Themen: Metaboliten & Metabolomics
Stichworte: LC-HRAM-MS/MS

Boosting compound identification confidence in Metabolomics by exploiting all available Q-TOF high resolution accurate mass spectral information.

Nikolas Kessler[1], Stephan Mävers[1], Frederik Walter[2], Marcus Persicke[2], Jörn Kalinowski[2], Matthias Szesny[1], Aiko Barsch[1], Heiko Neuweger[1]

[1]Bruker Daltonik GmbH, Deutschland; [2]Bielefeld University, Bielefeld, Deutschland; Matthias.szesny@bruker.com

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ID: 94 / Poster: 64
Poster
Themen: Metaboliten & Metabolomics
Stichworte: N-acyl homoserine lactones, quorum sensing, microscale synthesis, ionic liquid matrices, MALDI MS

Identification and quantification of N-acyl homoserine lactones involved in bacterial communication by matrix-assisted laser desorption/ionization mass spectrometry

Jan Leipert, Christian Treitz, Andreas Tholey

AG Systematische Proteomforschung & Bioanalytik, Institut für Experimentelle Medizin, Christian-Albrechts-Universität zu Kiel, Kiel, Deutschland; jan.leipert@stu.uni-kiel.de

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ID: 119 / Poster: 65
Poster
Themen: Metaboliten & Metabolomics
Stichworte: PIRL, Metabolomics, LC-MS/MS, FIA-MS/MS

Application of laser ablation for tissue metabolomics

Jonas Klein[1], Laura Heikaus[1], Gerrit Wolters-Eisfeld[1], Thomas Benninghaus[1], Nils-Owe Hansen[2], Dwayne Miller[2], Hartmut Schlüter[1]

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ID: 1 / Poster: 66
Poster
Themen: Metaboliten & Metabolomics, Organische Massenspektrometrie
Stichworte: Turnover of photopigments, 13C labelling, LC-MS, FTICR-MS

Quantitative turnover analysis of chlorophylls, carotenoids and tocopherol in green leaves by LC-MS and FTICR-MS

Björn Thiele, Andrea Neuwohner, Siegfried Jahnke, Ingar Janzik, Shizue Matsubara

IBG-2 Pflanzenwissenschaften, Forschungszentrum Jülich, Deutschland; b.thiele@fz-juelich.de

Poster-66-1.pdf

ID: 78 / Poster: 67
Poster
Themen: Metaboliten & Metabolomics, Organische Massenspektrometrie
Stichworte: phlorotannins, brown algae, LC-MS

Application of LC-MS technique for intra-thallus profiling of polyphenolics in three species of fucoid algae

Valeriia Lemesheva[1], Claudia Birkemeyer[2], Elena Tarakhovskaya[1]

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Poster-67-78.pdf

ID: 41 / Poster: 68
Poster

Themen: Metaboliten & Metabolomics, Sonstiges
Stichworte: Metabolomics, Chemical Profiling of Plant Extracts, Genotypes, Actaea racemosa

UPLC-ESI-QTOF-MS based chemical profiling of Actaea racemosa L. (black cohosh) rhizomes to investigate differences in cultivation, wild harvest, and genotypes

Marian Bittner[1], Andreas Springer[2], Regina Schenk[3], Matthias F. Melzig[1]
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Poster-68-41.pdf

ID: 158 / Poster: 69
Poster
Themen: Metaboliten & Metabolomics
Stichworte: MS based metabolite profiling strategies, metabolites, insects

Metabolomics to study the "war" between plants and insects - Systemic defense induction and post-ingestive rearrangement of plant toxins in insects.

Sven Heiling[1], Emmanuel Gaquerel[2], Aiko Barsch[3], Heiko Neuweger[3], Matthias Szesny[3], Ian T. Baldwin[1]
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ID: 156 / Poster: 70
Poster
Themen: Metaboliten & Metabolomics
Stichworte: Metabolomics

A step forward in GC-HRAM-MS based metabolomics - A novel atmospheric pressure GC-APCI Source increases quantitative and qualitative performance

Christian J. Wachsmuth[1], Aiko Barsch[2], Stephan Kühne[2], Peter J. Oefner[1], Katja Dettmer[1]
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ID: 209 / Poster: 71
Poster
Themen: Metaboliten & Metabolomics, Lebensmittelanalytik
Stichworte: Metabolomic Fingerprinting, Food Authenticity, UPLC-IMS-QToF, Foodomics

Discrimination of apple and potato cultivars by non-targeted metabolomic fingerprinting via UPLC-IMS-QToF analysis

Christin Claassen[1], Jasmin Wrage[1], Sascha Rohn[2], Jürgen Kuballa[1]
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Poster-71-209.pdf

ID: 128 / Poster: 72
Poster
Themen: Metaboliten & Metabolomics, Umweltanalytik
Stichworte: GC-MS, Metabolites, Anaerobic bio-degradation, Phenanthrene, TRIP

Metabolite analysis of the phenanthrene degrading, sulfate reducing bacterial enrichment culture (TRIP) using GC-MS

Zahra Farmani[1,2], Rainer U. Meckenstock[1], Wolfgang Schrader[2]
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Poster-72-128.pdf

ID: 82 / Poster: 73
Poster
Themen: Metaboliten & Metabolomics, Lebensmittelanalytik
Stichworte: Miniature mass spectrometry, food analysis, authentication, principal component analysis

Real-time food authentication with a miniature mass spectrometer

Stefanie Gerbig, Stephan Neese, Alexander Penner, Bernhard Spengler, Sabine Schulz
Justus-Liebig-Univeristät Gießen, Deutschland; stefanie.gerbig@anorg.chemie.uni-giessen.de

Poster-73-82.pdf

ID: 148 / Poster: 74
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging, MS - Informatik / Bioinformatik
Stichworte: imzML, Mass spectrometry imaging, MSI visualization tools, converters, public data repository

Overview of imzML-based software tools for MS imaging

Amol Fatangare, Nicolas Desbenoit, Andreas Römpp
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ID: 122 / Poster: 75
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging, Lipide & Lipidomics
Stichworte: MALDI MSI, Phospholipids, Ion suppression

Micro-arrays of faux tissue to investigate ion suppression effects in MALDI mass spectrometry of lipids

Marcel Boskamp[1], Fabian Eiersbrock[1], Marcel Wiegelmann[1], Klaus Dreisewerd[1,2], Jens Soltwisch[1,2]
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ID: 199 / Poster: 76
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging, Instrumentelle Entwicklungen
Stichworte: MALDI FT-ICR Imaging

MALDI FT-ICR Imaging: Double the Performance or Double the Samples using Quadrupolar Detection

Shannon Cornett[1], Christopher Thompson[1], Roland Jertz[3], Christoph Goseli[2], Claudia Kriete[3], Jochen Friedrich[3], Matthias Witt[3], Steve VanOrden[1], Michael Easterling[1], Christian Berg[1], Eugene Nikolaev[4], Arndt Asperger[3], Gökhan Baykut[3]
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ID: 194 / Poster: 77
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging
Stichworte: MRI contrast agents, mass spectrometry imaging, biological tissues

Mass Spectrometry Imaging as Tool for the Analysis of MRI Contrast Agents in Biological Tissues

Sabrina Trog[1], Ahmed El-Khatib[1], Hee-Jin Lee[1], Marcus R. Makowski[2], Sebastian Beck[1], Norbert Jakubowski[3], Michael W. Linscheid[1]
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Poster-77-194.pdf

ID: 234 / Poster: 78
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging, Proteine & Proteomics
Stichworte: DIVE, PIRL, laser ablation, proteome analysis, cell lysate collection

Optimized Biomolecular Extraction Using Desorption by Impulsive Vibrational Excitation: Applications to Embryonic Cell Differentiation

Johannes Kaub[1], Wesley D. Robertson[1], R. J. Dwayne Miller[1,2]
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ID: 232 / Poster: 79
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging, Instrumentelle Entwicklungen
Stichworte: mass spectrometry imaging, laser desorption ionization, infrared laser desorption

Development of Sub-Cellular Mass Spectrometry Imaging by Impulsive IR Laser Ablation

Frederik Busse[1], Wesley D. Robertson[1], R. J. Dwayne Miller[1,2]
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ID: 89 / **Poster: 80**
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging, Lipide & Lipidomics
Stichworte: MALDI-MSI, Lipidomics, Ionion suppression, MALDI-2

Towards qMALDI-MSI : MS imaging of phospholipids in mouse cerebellum followed by semi-quantitative nano-HPLC-ESI-MS of extracts from laser micro-dissected brain regions

Fabian Eiersbrock[1], Marcel Boskamp[1], Michael Mormann[1], Klaus Dreisewerd[1,2], Jens Soltwisch[1]
[1]Institute for Hygiene, University of Münster, Germany; [2]Interdisciplinary Center for Clinical Research (IZKF), University of Münster, Germany; f_eier01@wwu.de

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ID: 29 / **Poster: 81**
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging, Proteine & Proteomics
Stichworte: LA-ICP-MS, SDS-PAGE, Internal Standard, MeCAT

A new internal standard approach for laser ablation ICP-MS of polyacrylamide gels

René Becker, Jule Heimerl, Ahmed El-Khatib, Michael W. Linscheid
Humboldt-Universität zu Berlin, Institut für Chemie, Deutschland; rene.becker@hu-berlin.de

Poster-81-29.pdf

ID: 136 / **Poster: 82**
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging, MS - Informatik / Bioinformatik
Stichworte: MALDI Imaging, Raman Imaging, MS/Raman Data processing, imzML

Multimodal imaging combining mass spectrometry and vibrational spectroscopy using a single tissue section and an integrated data processing workflow

Rico Scheier, Nicholas Desbenoit, Axel Treu, Jasmin Kniese, Julia Kokesch-Himmelreich, Heinar Schmidt, Andreas Römpp
Universität Bayreuth, Deutschland; Axel.Treu@uni-Bayreuth.de

Poster-82-136.pdf

ID: 25 / **Poster: 83**
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging, Lebensmittelanalytik
Stichworte: MALDI-MSI, MS Imaging, Sclerotia, Mycotoxins, Ergot alkaloids

Localization of Ergot Alkaloids in Sclerotia of Claviceps purpurea by MALDI-MS Imaging

Simeon Vens-Cappell[1,2], Julian Dopstadt[3], Lisa Neubauer[4], Paul Tudzynski[4], Benedikt Cramer[3], Klaus Dreisewerd[1,2], Hans-Ulrich Humpf[3]
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ID: 100 / **Poster: 84**
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging, Instrumentelle Entwicklungen
Stichworte: MALDI-MSI, IR-MALDI, Postionization, Metabolites

CoolMALDI: Combination of IR-ablation and UV-postionization of snap-frozen tissue sections for sensitive imaging of lipids and metabolites

Jens Soltwisch[1,2], Hans Kettling[1,2], Simeon Vens-Cappell[1,2], Klaus Dreisewerd[1,2]
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ID: 96 / **Poster: 85**
Poster
Themen: Bildgebende Massenspektrometrie / MS Imaging
Stichworte: superbasic matrix DPN, AP-MALDI, AP-SMALDI-FT MSI, lipids, glucosinolates

Application of the Superbasic Matrix DPN in Atmospheric Pressure MALDI-MS-Analyses of Biological Samples

Jerrit Weissflog[1], Filip Kaftan[1], Aleš Svatoš[1,2]
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Poster-85-96.pdf

ID: 24 / Poster: 86
Poster
Themen: Sonstiges
Stichworte: Tandem MS, Oligonucleotides

Collision Specific Fragmentation of Oligonucleotides in Tandem Mass Spectrometry Experiments

Stefanie Ickert[1], Jens Riedel[1], Sebastian Beck[2], Michael Linscheid[2]
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Poster-86-24.pdf

ID: 15 / Poster: 87
Poster
Themen: Sonstiges
Stichworte: Pyridinderivate, REMPI-Spektroskopie, MATI-Spektroskopie, Anregungsenergien, Ionisationsenergien

REMPI- und MATI-Spektroskopie an den Methylpyridinen

Niklas Helle, Sascha Krüger, Jürgen Grotemeyer
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Poster-87-15.pdf

ID: 185 / Poster: 88
Poster
Themen: Sonstiges
Stichworte: ultra High Throughput Screening

Ultra High Throughput Drug Discovery Screening by MALDI-TOF Mass Spectrometry

Carl Haslam[1], Peter Marshall[1], Neil Hardy[1], Melanie Leveridge[1], Adrian Dunn[1], Meike Hamester[2], Jens Fuchser[2], Arne Fuetterer[2], Volker Sauerland[2], Arndt Asperger[2], Adrian Siemers[3], Swen Tyrasa[3], Debra Conway[3]
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ID: 151 / Poster: 89
Poster
Themen: Sonstiges
Stichworte: volatile analysis, mobile mass spectrometry, body odour sampling

The performance of mobile GC-MS for field sampling of body odours from common marmosets (Callithrix jacchus)

Marlen Kücklich[1], Manfred Möller[2], Andrea Marcillo[1], Almuth Einspanier[1], Anja Widdig[1,3,4], Claudia Birkemeyer[1]
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ID: 118 / Poster: 90
Poster
Themen: Glyco-Analytik & Glycomics, Native MS
Stichworte: Glycan analysis, middle down proteomics, In-Source-Fragmentation, Quantification

Analysis of human Glycoproteins with different LC-MS/MS and NMR techniques

Melissa Bärenfänger, Bernd Meyer
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Poster-90-118.pdf

ID: 87 / Poster: 91
Poster
Themen: Glyco-Analytik & Glycomics, Proteine & Proteomics
Stichworte: N-glycosylation, heterologous expression, nanoESI MS, CID

Identification of an unusual N-glycan detected in a tryptic glycopeptide derived from intergrin α7 expressed in Drosophila S2 cells

Julius Grosche[1], Johannes Eble[1], Michael Mormann[2], Gottfried Pohlentz[2]
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Poster-91-87.pdf

ID: 177 / Poster: 92
Poster
Themen: Glyco-Analytik & Glycomics, Proteine & Proteomics
Stichworte: O-glycosylation, GalNAc, VVA, enrichment

Mass spectrometric characterization of aberrant O-glycosylation in COSMC deficient mouse pancreas tissue

Benjamin Dreyer, Dennis Krösser, Pascal Steffen, Baris Mercanoglu, Gerrit Wolters-Eisfeld, Hartmut Schlüter
University Medical Center Hamburg Eppendorf, Deutschland; b.dreyer@uke.de

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ID: 101 / Poster: 93
Poster
Themen: Ionenmobilität, Glyco-Analytik & Glycomics
Stichworte: N-linked glycopeptides, N-linked glycoproteins

Increased confidence for the identification of N-linked glycopeptides using an optimised collision energy workflow

Gunnar Weibchen[1], Yi J Chen[2], Lee A Gethings[3], Alex Kuo[2], Yu-Ju Chen[2]
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Poster-93-101.pdf

ID: 166 / Poster: 94
Poster
Themen: MS - Informatik / Bioinformatik, Metaboliten & Metabolomics
Stichworte: HPLC, high resolution mass spectrometry, Metabolomics, MZmine 2, Algorithm

Algorithms for the annotation of isotopes, fragments and adducts, applied to HPLC-HRMS metabolomics data for the discovery of novel compounds

Robin Schmid[1,2], Birgit Arndt[1], Florian Hübner[1], Uwe Karst[2], Hans-Ulrich Humpf[1]
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Poster-94-166.pdf

ID: 167 / Poster: 95
Poster
Themen: MS - Informatik / Bioinformatik, Proteine & Proteomics
Stichworte: AGEs, GC-MS, glycation, metabolomics, microgravity, oxidative stress, seed germination, tandem mass spectrometry.

Simulated microgravity triggers transient enhancement of protein glycation and oxidation in germinating Brassica napus seeds

Veronika Chantseva[1], Anna Didio[2,3], Christian Ihling[4], Rico Schmidt[4], Galina Smolikova[1], Tatyana Grishina[3], Wolfgang Hoehenwarter[5], Andrej Frolov[2], Andrea Sinz[4], Sergei Medvedev[1], Tatiana Bilova[1,2]
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Poster-95-167.pdf

ID: 117 / Poster: 96
Poster
Themen: MS - Informatik / Bioinformatik, Proteine & Proteomics
Stichworte: bone healing, glycosaminoglycans, random forest modelling, SILAC

Comparative analysis of the effects of sulfated hyaluronic acid and dexamethasone on osteoblast differentiation by nanoLC-MS and random forest modeling.

Johannes R. Schmidt[1], Sarah Vogel[2], Stefan Kalkhof[3], Stephanie Möller[4], Martin von Bergen[1,5], Ute Hempel[2]
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Poster-96-117.pdf

ID: 147 / Poster: 97
Poster
Themen: MS - Informatik / Bioinformatik, Proteine & Proteomics
Stichworte: AGEs, aging, glycation, mass spectrometry, nodule, Phaseolus vulgaris, plant-microbial interaction, proteomics

Age-related formation of advanced glycation end products (AGEs) in root nodules of common beans (Phaseolus vulgaris)

Ahyoung Kim[1,2], Tatiana Bilova[1], Christian Ihling[3], Manuel Matamoros[4], Manuel Becana[4], Andrea Sinz[3], Ludger A. Wessjohann[1], Andrej Frolov[1]
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Poster-97-147.pdf

ID: 69 / Poster: 98
Poster
Themen: MS - Informatik / Bioinformatik
Stichworte: Elemental composition, accurate mass, isotope pattern

Determination of Molecular Formulas from Complex Isotope Pattern

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ID: 233 / Poster: 99
Poster
Themen: MS - Informatik / Bioinformatik, Proteine & Proteomics
Stichworte: Orbitrap, MS-cleavable cross-linkers

Optimization of crosslinked peptide analysis on an Orbitrap Fusion Lumos mass spectrometer

Ryan Bomgarden[1], Erum Raja[1], Chris Etienne[1], Fan Liu[4], Albert Heck[4], Mathias Müller[2], Rosa Viner[3]
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ID: 36 / Poster: 100
Poster
Themen: Ionenmobilität, Proteine & Proteomics
Stichworte: IMS, MRM, QconCAT, Proteomics, Lipidomics

IMS-DIA-MS Characterisation and IMS-MRM QconCAT Quantitation of the Lipidome and Apolipoprotein Complements of Obesity and Diabetes Cohorts

Marc Kipping[1], Lee A Gethings[2], Johannes PC Vissers[2], Jose Castro-Perez[3], Yvonne Woolerton[4], Lynn McLean[4], Robert Beynon[4], James Langridge[2]
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ID: 49 / Poster: 101
Poster
Themen: Ionenmobilität, Metaboliten & Metabolomics
Stichworte: derivatization, headspace gas chromatography, ion-mobility spectrometry, metabolomic fingerprinting

Derivatization of low-volatile compounds in aqueous solution and analysis by HS-GC-IMS

Alexander Roth, Fabian Simon, Vanessa König, Philipp Weller
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Poster-101-49.pdf

ID: 67 / Poster: 102
Poster
Themen: Ionenmobilität, Native MS
Stichworte: LILBID-MS, nESI, Ion Mobility, ATPase, ABC Transporter

Analyzing macromolecular complexes: subunit interactions of the F1F0 ATP synthase and conformational changes of the heterodimeric ABC transport complex TmrAB

Khanh Vu Huu, Stefan Brüchert, Robert Tampé, Volker Müller, Nina Morgner
Johann Wolfgang Goethe-Universität, Deutschland; VuHuu@chemie.uni-frankfurt.de
Poster-102-67.pdf

ID: 64 / Poster: 103
Poster
Themen: Ionenmobilität
Stichworte: Ion Mobility-Mass Spectrometry, Gas-Phase IR Spectroscopy, Human Islet Amyloid Polypeptide, Amyloid Intermediates

The Amyloid Formation Mechanism of Human IAPP: An Infrared Spectroscopy Approach

Waldemar Hoffmann[1], Michael T. Bowers[2], Gert von Helden[3], Kevin Pagel[1]
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ID: 28 / Poster: 104
Poster
Themen: Ionenmobilität, Lebensmittelanalytik
Stichworte: Authenticity assessment, Fingerprinting, Multivariate data analysis

Quality assessment of olive oil based on volatile compound fingerprinting using HRGC-IMS analysis

Natalie Gerhardt[1], Sascha Rohn[2], Philipp Weller[1]
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Poster-104-28.pdf

ID: 201 / Poster: 105
Poster
Themen: Organische Massenspektrometrie, Sonstiges
Stichworte: ageing, charcoal, extract, ESI-FTICRMS, soil

Historical charcoal additions potentially improve stability of soil organic carbon

Diana Hofmann[1], Bernhard Steffen[1], Hamada Abdelrahman[2], Ulrich Disko[1], Nele Meyer[3], Nils Borchard[4]
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Poster-105-201.pdf

ID: 6 / Poster: 106
Poster
Themen: Organische Massenspektrometrie, Sonstiges
Stichworte: MALDI-TOF-MS, Jeffamine, exakte Masse, Massenkalibrierung, Summenformel

Evaluierung basischer Polypropylenglycole als Standards zur internen Kalibrierung für exakte Massen in der positiv-Ionen MALDI-TOF-MS

Jürgen Gross
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ID: 237 / Poster: 107
Poster
Themen: Organische Massenspektrometrie
Stichworte: MALDI-MS, MALDI matrix, small molecules

CICCA-Tetrazole: An alternative matrix for the analysis of low molecular weight compounds by MALDI-MS

Anne Arnold, Michael Rühl, Michael Karas
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ID: 116 / Poster: 108
Poster
Themen: Organische Massenspektrometrie
Stichworte: Metaorganism, N-acyl homoserine lactone, quorum-sensing, quorum-quenching

Identification and characterization of N-acyl homoserine lactones by mass spectrometry

Christian Treitz[1], Cleo Pietschke[2], Sebastian Fraune[2], Andreas Tholey[1]
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ID: 221 / Poster: 109
Poster
Themen: Lebensmittelanalytik, Organische Massenspektrometrie
Stichworte: LC-MS/MS, Combined Fast Mode, Polarity Switching, Vitamins, Nutritional Supplements

Combined Fast Mode and Polarity Switching for Analysis of a Range of Vitamins and Nutritional Supplements in a Single Injection

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ID: 140 / Poster: 110
Poster
Themen: Lebensmittelanalytik, Organische Massenspektrometrie
Stichworte: Muscarine, normuscarine, diastereomeric separation, enantiomeric separation

Separation and identification of muscarine isomers

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Poster-110-140.pdf

ID: 17 / Poster: 111
Poster
Themen: Lebensmittelanalytik
Stichworte: SFE, SFC, LC-MS, GC-MS

Analysis of pesticides in food product using SFE-SFC-MSMS

Davor Fielitz[1], Sigrid Baumgarten[2]
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Poster-111-17.pdf

ID: 60 / Poster: 112
Poster
Themen: Lebensmittelanalytik
Stichworte: Folate, Stabilisotopenverdünnungsanalyse, LC-MS/MS, Validierung, Lebensmittel

Validierung einer Stabilisotopenverdünnungsanalyse von Folaten in Lebensmitteln und Bestimmung des Folatgehaltes in Naturprodukten

Nina Firl[1], Lisa Striegel[2], Christian Bunse[1], Michael Rychlik[2]
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Poster-112-60.pdf

ID: 155 / Poster: 113
Poster
Themen: Umweltanalytik, Lebensmittelanalytik
Stichworte: Environmental Contaminants

Simultaneous quantitation and confirmation of about 500 pesticide residues in food extracts using LC-QTOF accurate mass spectrometry

Petra Decker, Jochen Boosfeld, Karin Wendt, Carsten Baesmann
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ID: 188 / Poster: 114
Poster
Themen: Umweltanalytik
Stichworte: multiple polar pesticides

Parts-per-trillion level high-throughput quantitation of glyphosate, aminomethylphosponic acid (AMPA) and glufosinate in water samples by LC-MS/MS

Javier Lopez[1], Diego Martin[1], Cesar Perez[1], Jochen Boosfeld[2]
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ID: 230 / Poster: 115
Poster
Themen: Umweltanalytik
Stichworte: Fouier transform Orbitrap mass spectrometry, supercritical fluid extraction, crude oil, soil remediation

Supercritical fluid extraction as a soil remediation method for removal of crude oil related contaminations, analyzed by FT Orbitrap MS

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Poster-115-230.pdf

ID: 190 / Poster: 116
Poster
Themen: Umweltanalytik
Stichworte: VOCs, thermal desorption, GC-MS, XAD-2

Methodological aspects of mass spectrometric detection for profiling ambient VOCs with thermodesorption-GCMS

Andrea Marcillo[1], Arne Koch[1], Ilya Kozlov[1], Viktorija Jakimovska[4], Anja Widdig[1,2,3], Claudia Birkemeyer[1]
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Poster-116-190.pdf

ID: 165 / Poster: 117
Poster
Themen: Umweltanalytik, Sonstiges
Stichworte: Crude oil, Fenton reaction, supercritical CO2, Fourier transform Orbitrap mass spectrometry

Fenton based oxidation of crude oil in supercritical CO2

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Poster-117-165.pdf

ID: 197 / Poster: 118
Poster
Themen: Umweltanalytik, Organische Massenspektrometrie
Stichworte: Crude oil, fouling, ESI

Effect of temperature on crude oil fouling under inert and oxygenated conditions and subsequent analysis by HRMS

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Poster-118-197.pdf

ID: 183 / Poster: 119
Poster
Themen: Umweltanalytik, Organische Massenspektrometrie
Stichworte: Sulfamethoxazole, AOPs, photolysis, LC-HRMS

Investigations on the photolysis of sulfamethoxazole

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Poster-119-183.pdf

ID: 55 / Poster: 120
Poster
Themen: Native MS
Stichworte: Native MS, Ebola virus, nucleoprotein, self-assembly

Analyzing self-assembly of Ebola virus nucleoprotein with native mass spectrometry

Janine Kopicki[1], Johannes Heidemann[1], Cesar Muñoz-Fontela[1], Charlotte Uetrecht[1,2]
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Poster-120-55.pdf

ID: 10 / Poster: 121
Poster
Themen: Native MS
Stichworte: Native mass spectrometry, human noroviruses, glycan-mimetics, P domain, binding interactions.

Native mass spectrometry analysis of norovirus - glycan mimetics interaction

Hao Yan[1], Katharina Bücher[2], Laura Hartmann[2], Robert Creutznacher[3], Alvaro Mallagaray[3], Thomas Peters[3], Charlotte Uetrecht[1,4]

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Poster-121-10.pdf

ID: 93 / Poster: 122
Poster
Themen: Native MS
Stichworte: Membrane Proteins, Native-MS, LILBID-MS, Top-Down-MS

From Salty to Salt-free: Monitoring the Salt-dependent Dissoziation of the Membrane Protein Complex GCD in a Single Experiment

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ID: 52 / Poster: 123
Poster
Themen: Native MS
Stichworte: Native mass spectrometry (MS), viral cell entry, glycan binding, structural changes

Studying viral capsid glycan interaction with native MS

Ronja Pogan[1], Julia Lockhauserbäumer[1], Hao Yan[1], Grant Hansman[2], Mario Schelhaas[3], Bärbel Blaum[4], Charlotte Uetrecht[1,5]

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Poster-123-52.pdf

ID: 202 / Poster: 124
Poster
Themen: Proteine & Proteomics, Lebensmittelanalytik
Stichworte: AGEs, aging, amino acid analysis, glycation, LC-MS

Profiles of glycated amino acid adducts in the protein hydrolyzates of pea (Pisum sativum) seeds subjected to accelerated ageing

Maria Vikhnina[1,2], Alena Soboleva[1,2], Tahir Mehmood[1], Ekaterina Romanovskaya[2], Galina Smolikova[3], Andrej Frolov[1], Sergei Medvedev[3]

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Poster-124-202.pdf

ID: 146 / Poster: 125
Poster
Themen: Proteine & Proteomics, Organische Massenspektrometrie
Stichworte: DNA-protein cross-links, RNPxl, diepoxybutane, TiO2 enrichment

Analysis of 1,2,3,4-diepoxybutane induced DNA-histone cross-links by mass spectrometry

Katharina Mucek[1], Alexandra Stützer[1], Aleksander Chernev[1], Henning Urlaub[1,2]

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Poster-125-146.pdf

ID: 73 / Poster: 126
Poster
Themen: Proteine & Proteomics, Organische Massenspektrometrie
Stichworte: human immunodeficiency virus, ID-MS, viral load

Precise quantification of HIV proteins by isotope dilution mass spectrometry (ID-MS) for applications in HIV diagnostics

Luise Luckau[1], André Henrion[1], Petra Mischnick[2], Bernd Güttler[1]

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Poster-126-73.pdf

ID: 195 / Poster: 127
Poster
Themen: Proteine & Proteomics, Sonstiges
Stichworte: On-plate digestion, On-plate reduction and alkylation, Oxidation, Method development, MALDI-MS

Investigating on-plate digestion of proteins with regard to trypsin activity and oxidation

Michael Rühl, Stefan Schönborn, Ute Bahr, Michael Karas
Goethe-Universität Frankfurt am Main, Deutschland; ruehl@pharmchem.uni-frankfurt.de

Poster-127-195.pdf

ID: 210 / Poster: 128
Poster
Themen: Proteine & Proteomics, Sonstiges
Stichworte: Neurological biomarkers identification

Applying a Proteoform profiling method for neurological disorder biomarker discovery operations

Ulrike Burmester[1], Jerome Vialaret[2], Sylvain Lehmann[2], Audrey Gabelle[2,3], Pierre-Olivier Schmit[4], Christophe Hirtz[2]
[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Laboratoire de Biochimie et Protéomique Clinique, Institut de Médecine Régénératrice et de Biothérapie, CHU de Montpellier - Hôpital St. Eloi, Montpellier, France; [3]Centre Mémoire Ressources Recherche, CHU Montpellier, hôpital Gui de Chauliac, Montpellier, France; [4]Bruker Daltonique Wissembourg, France; ulrike.burmester@bruker.com

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ID: 204 / Poster: 129
Poster
Themen: Proteine & Proteomics
Stichworte: Galectin-3, affinity interaction, proteolytic extraction, mass spectrometry

CHARACTERIZATION OF CARBOHYDRATE BINDING SITES IN GALECTINS BY PROTEOLYTIC AFFINITY - MASS SPECTROMETRY

Yannick Baschung[1,2], Adrian Moise[3], Michael Przybylski[1]
[1]Steinbeis Centre Biopolymer Analysis & Biomedical Mass Spectrometry, Rüsselsheim, Germany; [2]Proteome Center, Institute of Immunology, University of Rostock, Rostock, Germany; [3]Department of Chemistry, University of Konstanz, Konstanz, Germany; yannick.baschung@hotmail.fr

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ID: 189 / Poster: 130
Poster
Themen: Proteine & Proteomics
Stichworte: Proteomics, Quantification, Label Free Quantification, Data Independent Acquisition

Comparison of label free quantification methods for proteomics

Dennis Krösser, Benjamin Dreyer, Pascal Steffen, Tobias Lange, Hartmut Schlüter
University Medical Center Hamburg-Eppendorf, Deutschland; d.kroesser@uke.de

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ID: 80 / Poster: 131
Poster
Themen: Proteine & Proteomics
Stichworte: Retinal guanylyl cyclase, cross-linking, GCAP, mass spectrometry

Structural Insights into Retinal Guanylyl Cyclase/GCAP-2 Interaction by Cross-linking and Mass Spectrometry

Anne Rehkamp, Tänzler Dirk, Christian Ihling, Andrea Sinz
Martin-Luther-University Halle-Wittenberg, Institute of Pharmacy, Department of Pharmaceutical Chemistry and Bioanalytics, Germany; anne.rehkamp@pharmazie.uni-halle.de

Poster-131-80.pdf

ID: 84 / Poster: 132
Poster
Themen: Proteine & Proteomics
Stichworte: Peptide Cross-Linking, (CID)-ESI-MS/MS, Protein structure analysis.

Synthesis of Isotope-Labeled Derivatives of the MS/MS-Cleavable Urea-Cross-Linker: Synthesis and Evaluation of Reactivity for Effective Protein Structure Analysis

Moritz Fischer[1], Christoph Hage[2], Mathias Schäfer[1], Andrea Sinz[2]

[1]Universität zu Köln, Deutschland; [2]Martin-Luther-Universität Halle-Wittenberg, Deutschland; mfisch11@smail.uni-koeln.de

Poster-132-84.pdf

ID: 98 / Poster: 133
Poster
Themen: Proteine & Proteomics
Stichworte: formate channel A, protein-interaction studies

Mass Spectrometry-Based Interaction Studies of the N-Terminus of the Formate Channel FocA from Escherichia coli

Jana Lorenz[1], Doreen Hunger[2], Gary Sawers[2], Andrea Sinz[1]
[1]Department of Pharmaceutical Chemistry and Bioanalytics, Institute of Pharmacy, Martin-Luther University Halle-Wittenberg, Halle (Saale), Germany; [2]Department of Microbiology, Institute of Biology, Martin-Luther University Halle-Wittenberg, Halle (Saale), Germany; jana.lorenz@pharmazie.uni-halle.de

Poster-133-98.pdf

ID: 215 / Poster: 134
Poster
Themen: Proteine & Proteomics
Stichworte: Beads, lysis, modification, extraction, preparation

A versatile method to extract, modify, enrich and digest proteomic samples directly from cell lysates

Yannik Lewin, Vahid Golghalyani, Michael Karas
Goethe Universität, Frankfurt, Deutschland; yannik.lewin@pharmchem.uni-frankfurt.de

Poster-134-215.pdf

ID: 175 / Poster: 135
Poster
Themen: Proteine & Proteomics
Stichworte: Quantitative Targeted Proteomics

Investigation of Q-TOF instruments advantages for label-free proteome analysis

Stephanie Kaspar-Schoenefeld, Markus Lubeck, Annette Michalski, Matthias Szesny, Pierre-Olivier Schmit
Bruker Daltonik GmbH, Deutschland; matthias.szesny@bruker.com

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ID: 62 / Poster: 136
Poster
Themen: Proteine & Proteomics
Stichworte: cross-linking, synaptic vesicles, protein complexes, protein interactions

Development of a protein interaction networks in synaptic vesicles using cross-linking and mass spectrometry

Sabine Wittig, Carla Schmidt
Interdisciplinary research center HALOmem, Martin Luther University Halle-Wittenberg, Kurt-Moses-Straße-3, 06120 Halle (Saale).; sabine.zurhorst@biochemtech.uni-halle.de

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ID: 91 / Poster: 137
Poster
Themen: Proteine & Proteomics
Stichworte: HDX-MS, PPARγ, phthalates, obesity

Phthalate metabolites MEHP and MEOHP but not the phthalate DEHP itself bind and activate the PPARγ

Isabel Kratochvil[1], Tommy Hofmann[1,2], Rita Schlichting[3], Beate Escher[3], Stefan Kalkhof[1,4], Martin von Bergen[1,5]
[1]Helmholtz-Centre for Environmental research (UFZ), Department of Molecular Systems Biology, Leipzig, Germany; [2]HALOmem, Halle (Saale), Germany; [3]Helmholtz-Centre for Environmental research (UFZ), Department of Cell Toxicology, Leipzig, Germany; [4]Coburg University, Department of Applied Sciences, Coburg, Germany; [5]University of Leipzig, Faculty of Biosciences, Pharmacy and Psychology, Leipzig, Germany; isabel.kratochvil@ufz.de

Poster-137-91.pdf

ID: 108 / Poster: 138
Poster
Themen: Proteine & Proteomics
Stichworte: T cell signaling, ADAP, Phosphorylation, Protein-Protein-Interaction

Analysis of serine-phosphorylation dependent protein-protein interactions of the T cell adaptor protein ADAP

Annika Manns[1], Michael Schümann[1], Heike Stephanowitz[1], Christian Freund[2], Eberhard Krause[1]
[1]Leibniz Institut für Molekulare Pharmakologie, Deutschland; [2]Institut für Chemie und Biochemie, Freie Universität Berlin, Deutschland; manns@fmp-berlin.de

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ID: 85 / Poster: 139
Poster
Themen: Proteine & Proteomics
Stichworte: 2D-LC, GelFree, high pH LC, Methanosarcina mazei, top-down

Combining 2D-LC-MS and Gelfree-LC-MS enhances both proteome coverage and the identification of short open reading frame encoded peptides

Liam Arron Cassidy[1], Daniela Prasse[2], Dennis Linke[1], Ruth A. Schmitz[2], Andreas Tholey[1]
[1]Div. Systematic Proteome Research & Bioanalytics, Institute for Experimental Medicine, Kiel University, Germany; [2]Institute for General Microbiology, Kiel University, Germany; l.cassidy@iem.uni-kiel.de

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ID: 245 / Poster: 140
Poster
Themen: Proteine & Proteomics
Stichworte: Differential centrifugation, SDS PAGE, in-gel digest, GeLC MS/MS analysis, label-free protein quantification

Improved protocol for recovery of vesicular proteins

Sofia Traikov, Nikolaj Zuleger, Henrik Thomas, Anna Shevchenko, Andrej Shevchenko
MPI of Cell Biology and Genetics, Dresden, Germany; traikov@mpi-cbg.de

Poster-140-245.pdf

ID: 113 / Poster: 141
Poster
Themen: Proteine & Proteomics
Stichworte: Quantitative Proteomics, 2D-LC MS, Isobaric Labeling, Alveolo-Capillary Barrier

Quantitative proteomics for the analysis of molecular changes in lung adenocarcinoma cells in response to Vitamin D3

Patrick Kaleja[1,2], Liam Cassidy[1], Sabine Fuchs[2], Andreas Tholey[1]
[1]AG Systematische Proteomforschung & Bioanalytik, Institut für Experimentelle Medizin, Christian-Albrechts-Universität, Kiel; [2]Klinik für Unfallchirurgie und Traumatologie, Experimentelle Unfallchirurgie, UKSH, Kiel; Kaleja.patrick@gmx.de

Poster-141-113.pdf

ID: 58 / Poster: 142
Poster
Themen: Proteine & Proteomics
Stichworte: SWATH, Micro Flow, Proteomics, Quantitation

Accelerating Data Independent Acquisition with Microflow Chromatography

Joerg Dojahn[1], Nick Morrice[2], Remco Van Soest[3], Christie Hunter[3]
[1]SCIEX, Deutschland; [2]SCIEX, UK; [3]SCIEX, USA; joerg.dojahn@sciex.com

Poster-142-58.pdf

ID: 220 / Poster: 143
Poster
Themen: Proteine & Proteomics
Stichworte: disulfide brigde reduction, biopharmaceuticals, antibodies, top-down MS

Evaluation of Optimal Conditions for Antibody Subunit Analysis on a Quadrupole-Orbitrap Mass Spectrometer

Kai Scheffler, Tabiwang Arrey, Martin Zeller, Eugen Damoc
Thermo Fisher Scientific, Deutschland; tabiwang.arrey@thermofisher.com

Poster-143-220.pdf

ID: 184 / Poster: 144
Poster
Themen: Proteine & Proteomics
Stichworte: Proteomics, Cold Stress, Plastids, Arabidopsis thaliana

Characterization of plastidal redox-responses during cold stress acclimation

Johannes Schütze, Hans-Peter Mock
IPK-Gatersleben, Deutschland; schuetzej@ipk-gatersleben.de

Poster-144-184.pdf

ID: 203 / Poster: 145
Poster
Themen: Proteine & Proteomics
Stichworte: Neo-glycoproteins, vaccine characterization, MALDI-MS, SPR

Innovative analytical methodologies for the development of new antitubercular agents

Francesca Rinaldi[1], Sara Tengattini[1], Caterina Temporini[1], Enrica Calleri[1], Gabriella Massolini[1], Loredana Lupu[2,3], Zdeněk Kukačka[2], Stefan Maeser[2], Michael Glocker[3], Michael Przybylski[2]
[1]Department of Drug Sciences, University of Pavia, Pavia, Italy; [2]Steinbeis Center for Biopolymer Analysis and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany; [3]Proteome Center, Institute of Immunology, University of Rostock, Rostock, Germany; francesca.rinaldi01@ateneopv.it

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ID: 135 / Poster: 146
Poster
Themen: Proteine & Proteomics
Stichworte: picosecond-infrared-laser, methionine oxidation, cancer, LC-MS/MS

Sampling of tissues with the picosecond-infrared-laser ablation for Redox Proteomics

Atef Mannaa[1], Marcel Kwiatkowski[1], Nils-Owe Hansen[2], R. J. Dwayne Miller[2], Hartmut Schlüter[1]
[1]Mass Spectrometric Proteomics, Department of Clinical Chemistry, University Medical Center Hamburg-Eppendorf, Hamburg, Germany.; [2]Max Planck Institute for the Structure and Dynamics of Matter, Atomically Resolved Dynamics Division, Luruper Chaussee 149, 22761 Hamburg, Germany.; atef.mannaa8@gmail.com

Poster-146-135.pdf

ID: 34 / Poster: 147
Poster
Themen: Proteine & Proteomics
Stichworte: post-translational modification, 2D gel electrophoresis, myelin, acetylome, tubulin acetylation

Partial Immunoblotting of 2D-Gels: A Novel Method to Identify Post-Translationally Modified Proteins Exemplified for the Myelin Acetylome

Kathrin Kusch[1], Marina Uecker[2], Thomas Liepold[2], Wiebke Möbius[1,3], Christian Hoffmann[4], Heinz Neumann[4], Hauke Werner[1], Olaf Jahn[2,3]
[1]Department of Neurogenetics, Max-Planck-Institute of Experimental Medicine, 37075 Göttingen, Germany; [2]Proteomics Group, Max-Planck-Institute of Experimental Medicine, 37075 Göttingen, Germany; [3]Center for Nanoscale Microscopy and Molecular Physiology of the Brain, 37075 Göttingen, Germany; [4]Free Floater (Junior) Research Group Applied Synthetic Biology, Georg-August University Göttingen, Institute for Microbiology and Genetics, 37077 Göttingen, Germany; jahn@em.mpg.de

Poster-147-34.pdf

19:30 - 23:59	**Konferenzdinner**

50. Jahrestagung der Deutschen Gesellschaft für Massenspektrometrie

Datum: Mittwoch, 08.03.2017

8:00 - 14:00	**Mi_Tag: Tagungsbüro**
8:30 - 8:35 **Hörsaal 3**	**Mi_Ank: Informationen**
8:35 - 9:20 **Hörsaal 3**	**Plenarvortrag 5: Biologische Massenspektrometrie** Chair der Sitzung: **Michael Karas**

ID: 236 / Plenarvortrag 5: 1
Plenarvortrag
Stichworte: shotgun lipidomics, blood plasma, lipid discovery, lipidomics software

Multifaceted Shotgun

Andrej Shevchenko
Max Planck Institute of Molecular Cell Biology and Genetics, Germany; shevchenko@mpi-cbg.de

9:20 - 10:05 **Hörsaal 3**	**Mi_Pr: DGMS-Preis für die Massenspektrometrie in den Biowissenschaften** Chair der Sitzung: **Wolf-Dieter Lehmann** Preisträger: K. Dreisewerd, Münster
10:25 - 10:30	**Kaffeepause 5**
10:30 - 12:30 **Hörsaal 1**	**MiV_1a: Proteine & Proteomics II** Chair der Sitzung: **Michael O. Glocker**

10:30 - 10:50
ID: 32 / MiV_1a: 1
Vortrag
Themen: Proteine & Proteomics
Stichworte: Pyrylium functionality, reliable fluorescent label, charge-tag for MS

Pyrylium-based dye and charge tagging in proteomics

Malte Bayer, Simone König
WWU Münster; malte.bayer@uni-muenster.de

MiV_1a-1-32.pdf

10:50 - 11:10
ID: 228 / MiV_1a: 2
Vortrag
Themen: Proteine & Proteomics
Stichworte: N-terminomics, Proteases, enrichment

Simple, scalable and sensitive tip-based enrichment of N-terminal peptides for profiling of protease substrates

Gerta Shema[1], Minh Nguyen[1], A. Saskia Venne[1], Steven Verhelst[1,2], René P. Zahedi[1]
[1]ISAS, Deutschland; [2]Department of Cellular and Molecular Medicine, Leuven, Belgium; rene.zahedi@isas.de

MiV_1a-2-228.pdf

11:10 - 11:30
ID: 222 / MiV_1a: 3
Vortrag
Themen: Proteine & Proteomics
Stichworte: Cleavable cross-linker, fragmentation, protein 3D-structures, protein-protein interactions, automated analysis

An Integrated Workflow for Structural Proteomics Studies based on Cross-linking/Mass Spectrometry with an MS/MS Cleavable Cross-linker

Christian Arlt[1], Michael Götze[2], Christian Ihling[1], Mathias Schäfer[3], Andrea Sinz[1]
[1]Institute of Pharmacy, Martin Luther University Halle-Wittenberg; [2]Institute of Biochemistry, Martin Luther University Halle-Wittenberg; [3]Institute for Organic Chemistry, Department of Chemistry, University of Cologne; christian.ihling@pharmazie.uni-halle.de

MiV_1a-3-222.pdf

11:30 - 11:50
ID: 186 / MiV_1a: 4
Vortrag
Themen: Proteine & Proteomics
Stichworte: Absolute quantification of proteins; GeLC-MS/MS; Western blotting; zebrafish embryogenesis

Absolute quantification of core histones in zebrafish embryos by MS Western

Mukesh Kumar[1], Shai R Joseph[1], Martina Augsburg[2], David Drechsel[1,3], Nadine Vastenhouw[1], Frank Buchholz[1,2], Marc Gentzel[1,4], Andrej Shevchenko[1]
[1]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany, Deutschland; [2]Medical Systems Biology Medical Faculty, TU Dresden, Dresden, Germany; [3]Present address: IMP Research Institute of Molecular Pathology, 1030 Vienna, Austria; [4]Present address: Center for Molecular and Cellular Bioengineering, TU Dresden, 01307 Germany; kumar@mpi-cbg.de

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11:50 - 12:10
ID: 216 / MiV_1a: 5
Vortrag
Themen: Proteine & Proteomics
Stichworte: ArgC, propionylation, shotgun proteomics, on bead digestion, amino modification

ArgC-like digestion: complementary or alternative to tryptic digestion?

Vahid Golghalyani, Moritz Neupärtl, Ilka Wittig, Ute Bahr, Michael Karas
Goethe-Universität-Frankfurt; g.vahid@gmail.com

12:10 - 12:30
ID: 43 / MiV_1a: 6
Vortrag
Themen: Proteine & Proteomics
Stichworte: Proteolysis, Factor XII, coagulation, LC-MS/MS, SDS-page

Proteome-wide detection of proteolysis in blood plasma by the SDS-PAGE-migration profile

Laura Heikaus de Figueiredo, Thomas Renné, Hartmut Schlüter
University Medical Center Hamburg Eppendorf, Deutschland; l.heikaus@uke.de

10:30 - 12:30
Hörsaal 2

MiV_2a: Grundlagen und Instrumentelle Entwicklungen II

Chair der Sitzung: **Jürgen Gross**

10:30 - 10:50
ID: 139 / MiV_2a: 1
Vortrag
Themen: Instrumentelle Entwicklungen, Glyco-Analytik & Glycomics
Stichworte: Gas-phase spectroscopy, oligosaccharides, isomers, glycoanalysis

Glycan Fingerprinting using Cold-Ion Infrared Spectroscopy

Eike Mucha[1,2], Ana Isabel Gonzalez Florez[2], Mateusz Marianski[2], Daniel A. Thomas[2], Waldemar Hoffmann[1,2], Weston B. Struwe[3], Heung Sik Hahm[4], Sandy Gewinner[2], Wieland Schöllkopf[2], Peter Seeberger[1,4], Gert von Helden[2], Kevin Pagel[1,2]
[1]Freie Universität Berlin, Deutschland; [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland; [3]Oxford Glycobiology Institute, Universität Oxford, Oxford, UK; [4]Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Potsdam, Deutschland; kevin.pagel@fu-berlin.de

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10:50 - 11:10
ID: 213 / MiV_2a: 2
Vortrag
Themen: Instrumentelle Entwicklungen, Sonstiges
Stichworte: Bitumen, direct-inlet-probe, time-of-flight-mass-spectrometry, high-resolution-mass-spectrometry, petroleum

The Usage of Direct Inlet Probe in combination with High Resolution Mass Spectrometry for the Characterization of Heavy Petroleum Products

Uwe Käfer[1], Christopher Rüger[2], Thomas Gröger[1], Jürgen Wendt[3], Thomas Wilharm[4], Ralf Zimmermann[1,2]
[1]Helmholtz Zentrum Muenchen, Neuherberg; [2]University of Rostock, Rostock; [3]LECO European Application & Technology Centre, Berlin; [4]ASG Analytik Service-Gesellschaft mbH, Neusäss; uwe.kaefer@helmholtz-muenchen.de

MiV_2a-2-213.pdf

11:10 - 11:30
ID: 21 / MiV_2a: 3
Vortrag

Themen: MS - Informatik / Bioinformatik, Grundlagen der Massenspektrometrie
Stichworte: FT-ICR, Resolution, FWHM, Mass/frequency filter

Power-function Resolution Filter in Fourier Transform Mass Spectrometry

Basem Kanawati[1], Theresa Bader[1], Karl Peter Wanczek[2], Yan Li[1], Philippe Schmitt-Kopplin[1,3]
[1]Helmholtz Zentrum München, Deutschland; [2]Universität Bremen; [3]Technische Universität München; basem.kanawati@helmholtz-muenchen.de

MiV_2a-3-21.pdf

11:30 - 11:50
ID: 226 / MiV_2a: 4
Vortrag
Themen: Instrumentelle Entwicklungen, Ionisationsmethoden
Stichworte: Instrumentation, ambient ionization, in-field mass spectrometry, DESI

Development of an autarkic desorption electrospray ionization source for in-field DESI-MS applications

Florian Lotz, Bernhard Spengler, Sabine Schulz
Justus-Liebig-Universität Gießen, Deutschland; florian.lotz@anorg.chemie.uni-giessen.de

MiV_2a-4-226.pdf

11:50 - 12:10
ID: 198 / MiV_2a: 5
Vortrag
Themen: Instrumentelle Entwicklungen
Stichworte: Innovations in Mass Spectrometry Instrumentation

2ω-FT-ICR Mass Spectrometry with Quadrupolar Detection

Roland Jertz[1], Christoph Gosteli[2], Walter Roeck[2], Claudia Kriete[1], Matthias Witt[1], Jochen Friedrich[1], Steve L. Van Orden[3], Christopher J. Thompson[3], Christian Berg[3], Jens Fuchser[1], Corinna Henkel[1], Michael L. Easterling[3], Eugene N. Nikolaev[4], Arndt Asperger[1], Gökhan Baykut[1]
[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Bruker BioSpin AG, Fällanden, Switzerland; [3]Bruker Daltonics Inc., Billerica, MA, USA; [4]Institute for Energy Problems of Chemical Physics, Russian Academy of Sciences, Moscow, Russia; jochen.friedrich@bruker.com

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12:10 - 12:30
ID: 125 / MiV_2a: 6
Vortrag
Themen: Instrumentelle Entwicklungen, Ionenmobilität
Stichworte: FAIMS, FTMS, APPI, isomer separation, crude oil

APPI-FAIMS-FTMS source and electrode optimization for the elucidation of structural features of crude oil constituents

Alessandro Vetere, Wolfgang Schrader
Max-Planck-Institut für Kohlenforschung, Deutschland; vetere@kofo.mpg.de

MiV_2a-6-125.pdf

10:30 - 12:30
Hörsaal 3

MiV_3a: Native Massespektrometrie

Chair der Sitzung: **Michael Linscheid**

10:30 - 10:50
ID: 79 / MiV_3a: 1
Vortrag
Themen: Native MS, Proteine & Proteomics
Stichworte: p53, MS/MS Cleavable Cross-linker, Stable Isotope Labeling, Native MS

An Integrated Mass Spectrometry Based Approach to Probe the Structure of the Full-Length Wild-Type Tetrameric p53 Tumor Suppressor

Christian Arlt, Christian Ihling, Andrea Sinz
Martin-Luther Universität Halle-Wittenberg, Deutschland; christian.arlt@pharmazie.uni-halle.de

MiV_3a-1-79.pdf

10:50 - 11:10
ID: 51 / MiV_3a: 2
Vortrag
Themen: Native MS
Stichworte: Native mass spectrometry, Nanodiscs, Membrane proteins

Applications of non-covalently bound membrane proteins in nanodiscs using LILBID-MS

Oliver Peetz, Jan Hoffmann, Nina Morgner

University of Frankfurt, Deutschland; peetz@chemie.uni-frankfurt.de

MiV_3a-2-51.pdf

11:10 - 11:30
ID: 211 / MiV_3a: 3
Vortrag
Themen: Native MS
Stichworte: Native MS, Protein-Lipid Interaction, Protein-Protein Interaction, Endocytosis

Structural characterization of protein-lipid complexes involved in clathrin-mediated endocytosis

Johannes Heidemann[1], Maria Marta Garcia Alai[2], Anna Gieras[2], Rob Meijers[2], Charlotte Uetrecht[1,3]
[1]Heinrich-Pette-Institute, Leibniz Institute for Experimental Virology, Hamburg, Germany; [2]European Molecular Biology Laboratory (EMBL), Hamburg, Germany; [3]European XFEL GmbH, Schenefeld, Germany; Johannes.Heidemann@hpi.uni-hamburg.de

MiV_3a-3-211.pdf

11:30 - 11:50
ID: 38 / MiV_3a: 4
Vortrag
Themen: Native MS
Stichworte: LILBID, beta-amyloid, oligomerisation, recombinant peptide, inhibitor screening

Steps towards a more native analysis of Aß42 using LILBID mass spectrometry

Tobias Lieblein[1], Tina Stark[1], Johnny Habchi[2], Michael Göbel[1], Michele Vendruscolo[2], Nina Morgner[1]
[1]Goethe-Universität Frankfurt, Deutschland; [2]University of Cambridge, United Kingdom; Lieblein@chemie.uni-frankfurt.de

MiV_3a-4-38.pdf

11:50 - 12:10
ID: 205 / MiV_3a: 5
Vortrag
Themen: Proteine & Proteomics
Stichworte: diatoms, biosilica, post-translational modification, polyamines

Polyamine modifications in biosilica-associated proteome

Alexander Milentyev[1], Christoph Heintze[2], Nicole Poulsen[2], Nils Kröger[2,3], Andrej Shevchenko[1]
[1]MPI-CBG, Dresden, Deutschland; [2]B-CUBE Center for Molecular Bioengineering, Dresden, Deutschland; [3]Department of Chemistry and Food Chemistry, Technische Universität Dresden, Deutschland; milentyev@mpi-cbg.de

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12:10 - 12:30
ID: 72 / MiV_3a: 6
Vortrag
Themen: Ionenmobilität, Native MS
Stichworte: Collision induced unfolding, ion mobility-mass spectrometry, native mass spectrometry, noncovalent protein-peptide complexes

Following the Unfolding and Dissociation of Calmodulin/Munc13 Complexes by Ion Mobility-Mass Spectrometry

Melanie Göth[1,2], Olaf Jahn[3], Kevin Pagel[1,2]
[1]Freie Universität Berlin, Deutschland; [2]Fritz-Haber-Institut Berlin, Deutschland; [3]Max-Planck-Institut für experimentelle Medizin, Göttingen, Deutschland; m.goeth@fu-berlin.de

12:30 - 13:00 **Hörsaal 3**	**Tagungsschluss** Prof.Dr. A. Sinz, DGMS Vorsitzende Prof. Dr. J. Grotemeyer, CAU Kiel Prof. Dr. D.A. Volmer, Saarbrücken

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Angelidou, Georgia	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig; Center for Biotechnology and Biomedicine, Universität Leipzig, Germany	Lipide I
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Armeni, Marina	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig; Center for Biotechnology and Biomedicine, Universität Leipzig, Germany	Lipide I
Arndt, Birgit	Institute of Food Chemistry, University of Münster, Germany	Poster Session Montag Abend
Arnhold, Jürgen	University of Leipzig, Medical Faculty, Institute of Medical Physics and Biophysics, Härtelstrasse 16- 18, 04107 Leipzig, Germany	Lipide II
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Baker, Erin	Pacific Northwest National Laboratory, USA	Ionen Mobilität
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Baldwin, Ian T.	Max Planck Institute for Chemical Ecology, Department for Molecular Ecology, Jena, Germany	Poster Session Montag Abend

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Barayeu, Uladzimir	University of Leipzig, Medical Faculty, Institute of Medical Physics and Biophysics, Härtelstrasse 16- 18, 04107 Leipzig, Germany	Lipide II Vortragend
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Barsch, Aiko	Bruker Daltonik GmbH, Deutschland	Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend
Bartelmus, Christian	Hoffmann la Roche AG, Schweiz	Poster Session Montag Abend Vortragend
Bartels, Benjamin	Research Group Mass spectrometry/Proteomics, Max Planck Institute for Chemical Ecology	Grundlagen und Instrumentelle Entwicklungen I Vortragend
Barth, Christof	Justus-Liebig-Universität Gießen, Deutschland	Poster Session Montag Abend Poster Session Montag Abend Vortragend
Baschung, Yannick	Steinbeis Centre Biopolymer Analysis & Biomedical Mass Spectrometry, Rüsselsheim, Germany; Proteome Center, Institute of Immunology, University of Rostock, Rostock, Germany	Poster Session Montag Abend Vortragend
Bauer, Anna	GALAB Laboratories GmbH, Deutschland	MS-Informatik/Bioinformatik
Baumgarten, Sigrid	Shimadzu Europa GmbH, Deutschland	Poster Session Montag Abend
Bayer, Malte	WWU Münster	Proteine & Proteomics II Vortragend
Baykut, Gökhan	Bruker Daltonik GmbH, Bremen, Germany	Grundlagen und Instrumentelle Entwicklungen II Poster Session Montag Abend
Becana, Manuel	Estación Experimental de Aula Dei, Consejo Superior de Investigaciones Científicas (CSIC), Department of Plant Nutrition	Poster Session Montag Abend
Becher, Simon	Institut für Anorganische und Analytische Chemie; Justus-Liebig-Universität Gießen	Poster Session Montag Abend
Beck, Florian	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Deutschland	Proteine & Proteomics I
Beck, Sebastian	Humboldt-Universität zu Berlin	Poster Session Montag Abend Poster Session Montag Abend
Becker, Alexander	Christian-Albrechts-Universität zu Kiel, Deutschland	Poster Session Montag Abend Vortragend
Becker, René	Humboldt-Universität zu Berlin, Institut für Chemie, Deutschland	Poster Session Montag Abend Vortragend
Begemann, Nora	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	Poster Session Montag Abend Vortragend
Beitz, Toralf	University of Potsdam, Germany	Poster Session Montag Abend
Benninghaus, Thomas	University Medical Center Hamburg-Eppendorf, Deutschland	Poster Session Montag Abend
Berg, Christian	Bruker Daltonics Inc., Billerica, MA, USA	Grundlagen und Instrumentelle Entwicklungen II Poster Session Montag Abend
Bergamini, Giovanna	Cellzome GmbH, Heidelberg	Proteine & Proteomics I
Bergmann, Julian	II physikalisches Insitut, Justus-Liebig-Universität Gießen, Deutschland	Poster Session Montag Abend Vortragend
Beynon, Robert	Centre for Proteome Research, Institute of Integrative Biology, University of Liverpool, Liverpool, UK	Poster Session Montag Abend
Bhandari, Dhaka ram	Justus Liebig University Giessen, Institute of Inorganic and Analytical Chemistry; Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, Heinrich-Buff-Ring 17, 35392 Giessen, Germany	Bildgebende Massenspektrometrie Metabolomics Vortragend
Bierstedt, Andreas	Bundesanstalt für Materialforschung und -prüfung, Deutschland	Poster Session Montag Abend Vortragend
Bilova, Tatiana	Leibniz-Institut für Pflanzenbiochemie, Abteilung Natur- und Wirkstoffchemie, Germany; Universität Leipzig, Fakultät für Chemie und	Analytische Anwendungen II Analytische Anwendungen II Vortragend Poster Session Montag Abend Poster Session Montag Abend

Autor(en)	Organisation(en)	Session
	Mineralogie, Germany; Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry (Halle/Saale); Faculty of Chemistry and Mineralogy, Universität Leipzig; Department of Plant Physiology and Biochemistry, St. Petersburg State University, Russia; Leibniz Institute of Plant Biochemistry, Department of Bioorganic Chemistry	
Birkemeyer, Claudia	Universität Leipzig, Fakultät für Chemie und Mineralogie, Germany; Faculty of Chemistry and Mineralogy, Universität Leipzig; Universität Leipzig, Deutschland	Analytische Anwendungen II Analytische Anwendungen II Ionisationsmethoden Poster Session Montag Abend Poster Session Montag Abend Vortragend Poster Session Montag Abend
Bittner, Marian	Freie Universität Berlin, Institute of Pharmacy, Pharmaceutical Biology	Poster Session Montag Abend Vortragend
Blaum, Bärbel	Interfaculty Institute of Biochemistry, University of Tübingen, Tübingen, Germany	Poster Session Montag Abend
Böcker, Sebastian	Chair for Bioinformatics, Friedrich Schiller University Jena	Grundlagen und Instrumentelle Entwicklungen I
Bomgarden, Ryan	Thermo Fisher Scientific, Rockford, IL, USA	Poster Session Montag Abend
Bookmeyer, Christoph H. M.	Institute for Hygiene, University of Münster, Robert-Koch-Str. 41, 48149 Münster, Germany	Poster Session Montag Abend Vortragend
Boosfeld, Jochen	Bruker Daltonik GmbH, Deutschland	Poster Session Montag Abend Vortragend Poster Session Montag Abend Vortragend
Borchard, Nils	Center for International Forestry Research, Indonesia	Poster Session Montag Abend
Borovinskaya, Olga	TOFWERK, Switzerland	Poster Session Montag Abend
Borowski, Kathrin	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	Poster Session Montag Abend
Boskamp, Marcel	Institute for Hygiene, University of Münster, Germany	Poster Session Montag Abend Poster Session Montag Abend Vortragend
Bowers, Michael T.	University of California, Santa Barbara, USA	Poster Session Montag Abend
Brandt, Wolfgang	Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry (Halle/Saale)	Analytische Anwendungen II
Brauch, Dominic	Faculty of Chemistry and Mineralogy, Universität Leipzig; Leibniz Institute of Plant Genetics and Crop Plant Research (Stadt Seeland)	Analytische Anwendungen II
Brockmann, Eike Ulrich	Institute for Hygiene, Biomedical Mass Spectrometry, University of Münster, Germany	Poster Session Montag Abend Vortragend
Brogly, Sophie	Hoffmann la Roche AG, Schweiz	Poster Session Montag Abend
Brosch, Mario	Department of Medicine I, University Medical Center Dresden, Technical University Dresden, Dresden, Germany	Lipide I
Brüchert, Stefan	Johann Wolfgang Goethe-Universität, Deutschland	Poster Session Montag Abend
Brügger, Britta	Biochemie-Zentrum Heidelberg, Deutschland	Lipide I Poster Session Montag Abend
Bruns, Heiko	University Hospital Erlangen, Deutschland	Metabolomics
Bücher, Katharina	Institute for Organic and Macromolecular Chemistry Heinrich-Heine-University Düsseldorf, Düsseldorf Germany	Poster Session Montag Abend
Buchholz, Frank	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany, Deutschland; Medical Systems Biology Medical Faculty, TU Dresden, Dresden, Germany	Proteine & Proteomics II
Bukowski, Nick	Markes International, Gwaun Elai Medi-Science Campus, Llantrisant, RCT, Wales, United Kingdom	Ionisationsmethoden
Bunse, Christian	Shimadzu Deutschland GmbH, Deutschland	Poster Session Montag Abend Vortragend

Autor(en)	Organisation(en)	Session
Burkhart, Julia M.	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Deutschland	Proteine & Proteomics I
Burmester, Ulrike	Bruker Daltonik GmbH, Deutschland	Poster Session Montag Abend Vortragend Poster Session Montag Abend Vortragend
Busse, Frederik	Max Planck Institut für Struktur und Dynamik der Materie, Hamburg, Deutschland	Poster Session Montag Abend Vortragend
Bussmann, Tanja	Research and Development, Beiersdorf AG, Hamburg	Poster Session Montag Abend
Butter, Falk	Institute of Molecular Biology, Deutschland	Analytische Anwendungen I Vortragend
Buzatto, Adriana	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster Session Montag Abend
Calleri, Enrica	Department of Drug Sciences, University of Pavia, Pavia, Italy	Poster Session Montag Abend
Campidelli, Stéphane	LICSEN, NIMBE, CEA, CNRS, Université Paris-Saclay, France	Gasphasenreaktionen & Fragmentierungen II
Cannistraci, Carlo V.	Biomedical Cybernetics Group, Biotechnology Center, Technical University Dresden, Dresden, Germany	Lipide I
Cassidy, Liam Arron	AG Systematische Proteomforschung & Bioanalytik, Institut für Experimentelle Medizin, Christian-Albrechts-Universität, Kiel	Poster Session Montag Abend Poster Session Montag Abend Vortragend
Castro-Perez, Jose	Waters Corporation, Milford, MA	Poster Session Montag Abend
Causon, Tim	BOKU Wien, Österreich	Ionen Mobilität Vortragend
Chait, Brian T.	The Rockefeller University, New York, USA	Wolfgang-Paul-Vortrag Vortragend
Chantseva, Veronika	Department of Plant Physiology and Biochemistry, St. Petersburg State University	Poster Session Montag Abend Vortragend
Chen, Yu-Ju	Academia Sinica, School of Chemistry, Taipei, Taiwan	Poster Session Montag Abend Poster Session Montag Abend
Chernev, Aleksandar	Max Planck Institute for Biophysical Chemistry, Göttingen, Germany	Analytische Anwendungen II Poster Session Montag Abend
Chervet, Jean-Pierre	ANTEC, Leyden	Poster Session Montag Abend
Ciucci, Sara	Biomedical Cybernetics Group, Biotechnology Center, Technical University Dresden, Dresden, Germany; Lipotype GmbH, Dresden, Germany	Lipide I
Claassen, Christin	GALAB Laboratories GmbH, Deutschland	Poster Session Montag Abend
Claude, Emmanuelle	Waters Corporation, United Kingdom	Bildgebende Massenspektrometrie
Clemen, Martin	Christian-Albrechts-Universität zu Kiel, Institut für Physikalische Chemie, Max-Eyth-Str. 1, 24118 Kiel, Deutschland	Gasphasenreaktionen & Fragmentierungen I Vortragend
Coliva, Giulia	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig; Center for Biotechnology and Biomedicine, Universität Leipzig, Germany	Lipide I Poster Session Montag Abend Vortragend
Colombo, Simone	Mass Spectrometry Centre, Department of Chemistry & QOPNA, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal	Poster Session Montag Abend
Coman, Cristina	Leibniz-Institut für Analytische Wissenschaften – ISAS e.V., Germany	Poster Session Montag Abend Vortragend
Conway, Debra	Analytik Jena AG, Jena, Germany	Poster Session Montag Abend
Cornett, Shannon	Bruker Daltonics, Billerica, MA, USA	Poster Session Montag Abend
Cramer, Benedikt	Institute of Food Chemistry, University of Münster, Germany	Poster Session Montag Abend
Crawford, Elizabeth	Saarland University, Saarbrücken, Deutschland	Analytische Anwendungen I Vortragend
Crecelius, Anna C.	Friedrich Schiller University Jena, Deutschland	Analytische Anwendungen I Vortragend
Creutznacher, Robert	Institute of Chemistry, University of Lübeck, Lübeck, Germany	Poster Session Montag Abend
Crone, Barbara	Institut für Anorganische und Analytische Chemie, Universität Münster, Deutschland	Bildgebende Massenspektrometrie Vortragend
Czech, Hendryk	Universität Rostock, Deutschland	Ionisationsmethoden Vortragend

Autor(en)	Organisation(en)	Session
Damoc, Eugen	Thermo Fisher Scientific, Deutschland	Poster Session Montag Abend Poster Session Montag Abend
Danne-Rasche, Niklas	Leibniz Institut für Analytische Wissenschaften ISAS e.V.	Lipide I Vortragend
Danquah, Bright D.	Proteome Center Rostock, Deutschland	Ionen Mobilität
Danz, Norbert	Fraunhofer Institute for Applied Optics and Precision Engineering IOF	Grundlagen und Instrumentelle Entwicklungen I
Darland, Ed	Agilent Technologies, Santa Clara, USA	Ionen Mobilität
De Angelis, Francesco	Dipart. di Sci. Fisiche e Chimiche, Università degli Studi dell'Aquila, Via Vetoio, Coppito, 67100 L'Aquila, Italy	Gasphasenreaktionen & Fragmentierungen I
de Bruyn, René	Netherlands Forensic Institute, Forensic Chemistry – Chemical Identification Analysis, 2497 GB The Hague, Netherlands	Analytische Anwendungen I
Decker, Petra	Bruker Daltonik GmbH, Deutschland	Poster Session Montag Abend
Dedishov, Ruslan	Markes International GmbH, Schleussnerstrasse 42, Frankfurt, Germany	Ionisationsmethoden
Dell'Aica, Margherita	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Deutschland	Proteine & Proteomics I
Denno, Yvonne	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	Poster Session Montag Abend
Desbenoit, Nicholas	Universität Bayreuth, Deutschland	Poster Session Montag Abend
Desbenoit, Nicolas	Chair of Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth, Germany	Poster Session Montag Abend Bildgebende Massenspektrometrie
Dettmer, Katja	University of Regensburg, Institute of Functional Genomics, Regensburg, Deutschland	Poster Session Montag Abend
Diarra, David	Oil-Wärme-Institut GmbH, Herzogenrath, Deutschland	Poster Session Montag Abend
Dickel, Timo	II physikalisches Insitut, Justus-Liebig-Universität Gießen, Deutschland; GSI Darmstadt, Deutschland	Poster Session Montag Abend
DiConza, Giusy	Laboratory of Molecular Oncology and Angiogenesis, Vesalius Research Center, Leuven, Belgium	Klinische Diagnostik & Forensic
Didio, Anna	Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry; Department of Biochemistry, St. Petersburg State University	Poster Session Montag Abend
Dietrich, Dörthe	Westfälische Wilhelms-Universität Münster	Bildgebende Massenspektrometrie Vortragend
Ding, Xuelu	Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen	Ionisationsmethoden Vortragend
Dinse, Martin	PerkinElmer LAS (Germany) GmbH, Deutschland	Poster Session Montag Abend Vortragend
Dirk, Tänzler	Martin-Luther-University Halle-Wittenberg, Institute of Pharmacy, Department of Pharmaceutical Chemistry and Bioanalytics, Germany	Poster Session Montag Abend
Disko, Ulrich	Forschungszentrum Jülich, Deutschland	Poster Session Montag Abend
Dojahn, Joerg	SCIEX, Deutschland	Poster Session Montag Abend Vortragend
Domingues, M. Rosario	Mass Spectrometry Centre, Department of Chemistry & QOPNA, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal	Poster Session Montag Abend
Domingues, Pedro	Mass Spectrometry Centre, Department of Chemistry & QOPNA, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal	Poster Session Montag Abend
Dopstadt, Julian	Institute of Food Chemistry, University of Münster, Germany	Poster Session Montag Abend
Dral, Pavlo O.	Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany	Gasphasenreaktionen & Fragmentierungen II

Autor(en)	Organisation(en)	Session
Drechsel, David	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany, Deutschland; Present address: IMP Research Institute of Molecular Pathology, 1030 Vienna, Austria	Proteine & Proteomics II
Dreger, Mathias	caprotec bioanalytics GmbH	Proteine & Proteomics I
Dreisewerd, Klaus	Institute for Hygiene, University of Münster, Germany; Interdisciplinary Center for Clinical Research (IZKF), University of Münster, Germany; University of Münster, Institute of Hygiene, Biomedical Mass Spectrometry, Germany; Institute for Hygiene, University of Münster, Robert-Koch-Str. 41, 48149 Münster, Germany	Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend Grundlagen und Instrumentelle Entwicklungen I Poster Session Montag Abend Poster Session Montag Abend
Drewello, Thomas	Friedrich-Alexander-University Erlangen-Nürnberg, Germany	Gasphasenreaktionen & Fragmentierungen II Gasphasenreaktionen & Fragmentierungen II Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend
Dreyer, Benjamin	University Medical Center Hamburg Eppendorf, Deutschland	Poster Session Montag Abend Vortragend Poster Session Montag Abend
Dülcks, Thomas	Universität Bremen, Deutschland	Poster Session Montag Abend Vortragend
Dunn, Adrian	Departments of Platform Technology & Science, GlaxoSmithKline, Stevenage, UK	Poster Session Montag Abend
Dürr, Maximilian	Friedrich-Alexander-University Erlangen-Nürnberg, Deutschland	Poster Session Montag Abend
Duschl, Wolfgang J.	Christian-Albrechts-Universität zu Kiel, Deutschland	„Ja wo seid Ihr denn alle? Von der (seriösen) Suche nach extraterrestrischem Leben“ Vortragend
Dwayne Miller, R. J.	Max Planck Institute for the Structure and Dynamics of Matter CFEL, Hamburg	Poster Session Montag Abend
Easterling, Michael L.	Bruker Daltonics, Billerica, MA, USA	Poster Session Montag Abend Grundlagen und Instrumentelle Entwicklungen II
Eble, Johannes	Institut für Physiologische Chemie und Pathobiochemistry, Universität Münster, Deutschland	Poster Session Montag Abend
Eckelmann, Paula	Federal Criminal Police Office, Forensic Institute, 65193 Wiesbaden, Germany; Justus-Liebig-University Giessen, Institute of Food Chemistry and Food Biotechnology, 35392 Giessen, Germany	Analytische Anwendungen I
Eckey, Kevin	Universität Münster, Deutschland	Poster Session Montag Abend Vortragend
Edler, Stefan	LAS Perkinelmer GmbH, Deutschland	Poster Session Montag Abend Vortragend
Eggers, Lars Florian	Research Center Borstel, Division of Bioanalytical Chemistry, Parkallee 1-40, D-23845 Borstel, Germany.	Lipide II Vortragend
Eggert, Dennis	Heinrich Pette Institute, Leibniz Institute for Experimental Virology, Hamburg	Poster Session Montag Abend
Eiersbrock, Fabian	Institute for Hygiene, University of Münster, Germany	Poster Session Montag Abend Vortragend Poster Session Montag Abend
Einspanier, Almuth	Universität Leipzig, Deutschland	Poster Session Montag Abend
El-Khatib, Ahmed	Humboldt-Universität zu Berlin, Institut für Chemie, Deutschland	Poster Session Montag Abend Poster Session Montag Abend
Enders, Claudia	Merck KGaA, Frankfurter Str. 250, 64293 Darmstadt, Germany	Poster Session Montag Abend
Engeser, Marianne	Universität Bonn, Deutschland	Gasphasenreaktionen & Fragmentierungen II Vortragend Poster Session Montag Abend
Ermler, Ulrich	Max Planck Institute of Biophysics, Frankfurt	Poster Session Montag Abend
Esch, Patrick	Institute of Inorganic and Analytical Chemistry, Justus-Liebig-University, Giessen, Germany	Lipide I Vortragend

Autor(en)	Organisation(en)	Session
Escher, Beate	Helmholtz-Centre for Environmental research (UFZ), Department of Cell Toxicology, Leipzig, Germany	Poster Session Montag Abend
Esfeld, Sonja	University Hospital Essen, Medical Faculty, West German Heart and Vascular Center, Department of Cardiology and Department of Angiology, Germany	Poster Session Montag Abend
Etienne, Chris	Thermo Fisher Scientific, Rockford, IL, USA	Poster Session Montag Abend
Faelth-Savitski, Maria	Cellzome GmbH, Heidelberg	Proteine & Proteomics I
Fagbadebo, Funmilayo	Leibniz-Institut für Pflanzenbiochemie, Abteilung Natur- und Wirkstoffchemie, Germany	Analytische Anwendungen II
Farmani, Zahra	Bio-film Center Universität Duisburg-Essen; Max-Planck-Institut für Kohlenforschung, Germany	Poster Session Montag Abend Vortragend
Fatangare, Amol	Chair of Bioanalytical Sciences and Food Analysis, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth, Germany	Bildgebende Massenspektrometrie Poster Session Montag Abend Vortragend
Fazel, Ramin	The University of Tehran, Iran; Universitätsklinikum Hamburg-Eppendorf, Germany	Analytische Anwendungen II Vortragend
Fedorova, Maria	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig, Germany; Center for Biotechnology and Biomedicine, Universität Leipzig, Germany	Poster Session Montag Abend Lipide I Vortragend Poster Session Montag Abend
Fiedler, Dorothea	Leibniz-Institut für molekulare Pharmakologie (FMP), Deutschland; Humboldt-Universität zu Berlin; Princeton University	Proteine & Proteomics I
Fielitz, Davor	Shimadzu Deutschland GmbH, Deutschland	Poster Session Montag Abend Vortragend
Firl, Nina	Shimadzu Deutschland GmbH, Deutschland	Poster Session Montag Abend
Fischer, Michael	Helmholtz-Zentrum München,Deutschland	Poster Session Montag Abend
Fischer, Moritz	Universität zu Köln, Deutschland	Poster Session Montag Abend Vortragend
Fischle, Wolfgang	Max Planck Institute for Biophysical Chemistry, Göttingen, Germany; KAUST, Saudi Arabia	Analytische Anwendungen II
Fjeldsted, John	Agilent Technologies, Santa Clara, USA	Ionen Mobilität
Flemmig, Jörg	University of Leipzig, Medical Faculty, Institute of Medical Physics and Biophysics, Härtelstrasse 16- 18, 04107 Leipzig, Germany	Lipide II
Folberth, Julica	University of Lübeck, Germany	Metabolomics Vortragend
Franken, Holger	Cellzome GmbH, Heidelberg	Proteine & Proteomics I
Franz, Florian	Universitätsklinikum Freiburg, Institut für Rechtsmedizin, Forensische Toxikologie, Germany	Poster Session Montag Abend
Franzke, Joachim	Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V.	Ionisationsmethoden
Fraune, Sebastian	Zoologisches Institut, Uni Kiel	Poster Session Montag Abend
Frensemeier, Lisa	Universität Münster, Deutschland	MS Analytik Vortragend
Freund, Christian	Institut für Chemie und Biochemie, Freie Universität Berlin, Deutschland	Poster Session Montag Abend
Friedrich, Jochen	Bruker Daltonik GmbH, Bremen, Germany	Grundlagen und Instrumentelle Entwicklungen II Vortragend Poster Session Montag Abend
Frolov, Andrej	Leibniz-Institut für Pflanzenbiochemie, Abteilung Natur- und Wirkstoffchemie, Germany; Universität Leipzig, Fakultät für Chemie und Mineralogie, Germany	Analytische Anwendungen II Vortragend
Frolov, Andrej	Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry (Halle/Saale); Faculty of Chemistry and Mineralogy, Universität Leipzig;	Analytische Anwendungen II Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend

Autor(en)	Organisation(en)	Session
	Leibniz Institute of Plant Biochemistry, Department of Bioorganic Chemistry	
Fuchs, M.	2Joint Mass Spectrometry Centre Helmholtz-Zentrum München, Comprehensive Molecular Analytics (CMA), Neuherberg, Germany	Poster Session Montag Abend
Fuchs, Sabine	Klinik für Unfallchirurgie und Traumatologie, Experimentelle Unfallchirurgie, UKSH, Kiel	Poster Session Montag Abend
Fuchser, Jens	Bruker Daltonik GmbH, Bremen, Germany	Grundlagen und Instrumentelle Entwicklungen II Poster Session Montag Abend
Fuetterer, Arne	Bruker Daltonik GmbH, Germany	Poster Session Montag Abend
Fufezan, Christian	Institute for Biology and Biotechnology of Plants, University Münster, Münster, Germany;	Proteine & Proteomics I
Fuh, Marceline Manka	University Medical Centre Hamburg-Eppendorf, Institute of Clinical Chemistry, Department for Mass Spectrometric Proteomics, Hamburg Germany	Poster Session Montag Abend Vortragend
Furrer, Julien	Department of Chemistry and Biochemistry, University of Bern	Poster Session Montag Abend
Gabelica, Valérie	Inserm, CNRS, Université de Bordeaux, Laboratoire "Acides Nucléiques, Régulations Naturellee et Artificielle" (ARNA, U1212, UMR5320), IECB, Pessac, France	“Nucleic acids biophysics" Vortragend
Gabelle, Audrey	Laboratoire de Biochimie et Protéomique Clinique, Institut de Médecine Régénératrice et de Biothérapie, CHU de Montpellier - Hôpital St. Eloi, Montpellier, France; Centre Mémoire Ressources Recherche, CHU Montpellier, hôpital Gui de Chauliac, Montpellier, France	Poster Session Montag Abend
Gade, Stephan	Cellzome GmbH, Heidelberg	Proteine & Proteomics I
Gallaspy, Alan	PerkinElmer LAS (Germany) GmbH, Deutschland	Poster Session Montag Abend
Galyamova, Aigerim	Pennsylvania State University, USA	Ionisationsmethoden
Gambaryan, Stepan	Sechenov Institute of Evolutionary Physiology and Biochemistry, Russian Academy of Sciences, Saint Petersburg, Russia;	Proteine & Proteomics I
Gaquerel, Emmanuel	Centre for Organismal Studies Heidelberg, University of Heidelberg, Germany	Poster Session Montag Abend
Garbeva, Paolina	Department of Microbial Ecology, Netherlands Institute of Ecology, Wageningen, The Netherlands	Metabolomics
Garcia Alai, Maria Marta	European Molecular Biology Laboratory (EMBL), Hamburg, Germany	Native Massespektrometrie
Geiger, Jörg	Interdisciplinary Bank of Biomaterials and Data, Würzburg, Germany;	Proteine & Proteomics I
Geissel, Hans	II physikalisches Insitut, Justus-Liebig-Universität Gießen, Deutschland; GSI Darmstadt, Deutschland	Poster Session Montag Abend
Gentzel, Marc	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany, Deutschland; Present address: Center for Molecular and Cellular Bioengineering, TU Dresden, 01307 Germany	Proteine & Proteomics II
Gerbig, Stefanie	Justus Liebig University, Gießen, Deutschland	Analytische Anwendungen I Poster Session Montag Abend Vortragend
Gerbig, Stefanie	Justus-Liebig-Universität Gießen, Institut für Anorganische und Analytische Chemie	Analytische Anwendungen I
Gerhardt, Natalie	Hochschule Mannheim, Deutschland	Poster Session Montag Abend Vortragend
Gethings, Lee	Waters Corporation, Wilmslow, United Kingdom	Poster Session Montag Abend Poster Session Montag Abend
Gethings, Lee A	Waters, Wilmslow, UK	Poster Session Montag Abend Poster Session Montag Abend

Autor(en)	Organisation(en)	Session
Gewinner, Sandy	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland	Grundlagen und Instrumentelle Entwicklungen II
Gieras, Anna	European Molecular Biology Laboratory (EMBL), Hamburg, Germany	Native Massespektrometrie
Glocker, Michael	Proteome Center, Institute of Immunology, University of Rostock, Rostock, Germany	Poster Session Montag Abend
Glocker, Michael O.	Proteome Center Rostock, Deutschland	Ionen Mobilität Vortragend
Göbel, Michael	Goethe-Universität Frankfurt, Deutschland	Native Massespektrometrie
Goldmann, Torsten	Pathology of the University Hospital of Lübeck and the Research Center Borstel, Clinical and Experimental Pathology, 23538 Lübeck and 23845 Borstel, Germany.; Airway Research Center North, German Center for Lung Research, Wöhrendamm 80, 22927 Großhansdorf, Germany	Lipide II
Golghalyani, Vahid	Goethe-Universität-Frankfurt	Proteine & Proteomics II Vortragend Poster Session Montag Abend
Gonzalez Florez, Ana Isabel	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland	Grundlagen und Instrumentelle Entwicklungen II
Goseli, Christoph	Bruker BioSpin, Fällanden, Switzerland	Poster Session Montag Abend
Gosteli, Christoph	Bruker BioSpin AG, Fällanden, Switzerland	Grundlagen und Instrumentelle Entwicklungen II
Göth, Melanie	Freie Universität Berlin, Deutschland; Fritz-Haber-Institut Berlin, Deutschland	Native Massespektrometrie Vortragend
Gottfried, Sebastian	Waters Corporation, United Kingdom	Bildgebende Massenspektrometrie Vortragend
Gottwald, Sven	Department of Plant Breeding, Justus Liebig University Giessen, Heinrich-Buff-Ring 26–32, 35392 Giessen, Germany	Metabolomics
Götze, Michael	Institute of Biochemistry, Martin Luther University Halle-Wittenberg	Proteine & Proteomics II
Grafinger, Katharina	Universtität Bern, Institut für Rechtsmedizin, Forensische Toxikologie und Chemie, Switzerland	Poster Session Montag Abend Vortragend
Grevelding, Christoph	Justus-Liebig-Universität Gießen, Institut für Parasitologie	Analytische Anwendungen I
Grishina, Tatiana	Universität St. Petersburg, Lehrstuhl Biochemie, Russia; Department of Biochemistry, St. Petersburg State University	Analytische Anwendungen II Poster Session Montag Abend
Groessl, Michael	Tofwerk, Uttigenstrasse 22, CH-3600 Thun, Switzerland	Ionen Mobilität Poster Session Montag Abend
Gröger, Thomas	Helmholtz Zentrum Muenchen, Neuherberg	Grundlagen und Instrumentelle Entwicklungen II
Grosche, Julius	Institut für Physiologische Chemie und Pathobiochemistry, Universität Münster, Deutschland	Poster Session Montag Abend
Gross, Jürgen	Universität Heidelberg, Deutschland	Poster Session Montag Abend Vortragend
Grotemeyer, Jürgen	Christian-Albrechts-Universität zu Kiel, Institut für Physikalische Chemie, Max-Eyth-Str. 1, 24118 Kiel, Deutschland; Christian-Albrechts-Universität zu Kiel, Deutschland	Gasphasenreaktionen & Fragmentierungen I Gasphasenreaktionen & Fragmentierungen II Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend
Gruber, Uschi	caprotec bioanalytics GmbH	Proteine & Proteomics I
Grübner, Isabell	Goethe Universität Frankfurt, Deutschland	Poster Session Montag Abend
Grutters, Michiel	Netherlands Forensic Institute, Forensic Chemistry – Chemical Identification Analysis, 2497 GB The Hague, Netherlands	Analytische Anwendungen I
Grützmacher, Hans-Friedrich	Department of Chemistry, Bielefeld University	Poster Session Montag Abend Poster Session Montag Abend
Güttler, Bernd	Physikalisch-Technische-Bundesanstalt, Deutschland	Poster Session Montag Abend
Habchi, Johnny	University of Cambridge, United Kingdom	Native Massespektrometrie
Hachenberger, Yves U.	Humboldt-Universität zu Berlin	Poster Session Montag Abend Vortragend

Autor(en)	Organisation(en)	Session
Hachmöller, Oliver	Institute of Inorganic and Analytical Chemistry, University of Münster, Münster, Germany	MS Analytik Vortragend
Hädener, Marianne	University of Bern, Institute of Forensic Medicine, Forensic Toxicology and Chemistry, Bühlstrasse 20, 3012 Bern, Switzerland	Poster Session Montag Abend Vortragend
Hage, Christoph	Martin-Luther-Universität Halle-Wittenberg, Deutschland	Gasphasenreaktionen & Fragmentierungen II Vortragend Poster Session Montag Abend
Hagenhoff, Sebastian	Westfälische Wilhelms-Universität Münster	Ionisationsmethoden Vortragend
Hahm, Heung Sik	Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Potsdam, Deutschland	Grundlagen und Instrumentelle Entwicklungen II
Hahn, Bill	PerkinElmer LAS (Germany) GmbH, Deutschland	Poster Session Montag Abend
Hahn, Stefanie	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	Poster Session Montag Abend
Hahn, Uwe	Universidad Autónoma de Madrid, Spain; University of Strasbourg and CNRS, European School for Chemistry, Polymers and Materials (ECPM), France	Poster Session Montag Abend
Hakelberg, Matthias	caprotec bioanalytics GmbH	Proteine & Proteomics I
Hamester, Meike	Bruker Daltonik GmbH, Germany	Poster Session Montag Abend
Han, Wei	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster Session Montag Abend
Hann, Stephan	BOKU Wien, Österreich	Ionen Mobilität
Hannich, Thomas	University of Geneva, Department of Biochemistry	Bildgebende Massenspektrometrie
Hansen, Nils-Owe	Max Planck Institute for the Structure and Dynamics of Matter	Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend
Hansman, Grant	DKFZ and Department of Infectious Diseases and Virology University of Heidelberg, Heidelberg, Germany	Poster Session Montag Abend
Hardy, Neil	Departments of Platform Technology & Science, GlaxoSmithKline, Stevenage, UK	Poster Session Montag Abend
Hart, Philippa J.	Waters Corporation, United Kingdom	Bildgebende Massenspektrometrie
Hartmann, Laura	Institute for Organic and Macromolecular Chemistry Heinrich-Heine-University Düsseldorf, Düsseldorf Germany	Poster Session Montag Abend
Haslam, Carl	Departments of Platform Technology & Science, GlaxoSmithKline, Stevenage, UK	Poster Session Montag Abend
Hayen, Heiko	Westfälische Wilhelms-Universität Münster	Ionisationsmethoden Poster Session Montag Abend
Hayen, Heiko	WWU Münster, Deutschland; Westfälische Wilhelms-Universität Münster, Deutschland	Metabolomics Poster Session Montag Abend
Heber, Volker	PerkinElmer, Deutschland	Poster Session Montag Abend Vortragend
Heck, Albert	Universiteit Utrecht, The Netherlands	Poster Session Montag Abend
Heemskerk, Johan W. M.	Department of Biochemistry, Cardiovascular Research Institute Maastricht, Maastricht University, The Netherlands;	Proteine & Proteomics I
Heeren, Ron M.A.	Maastricht University, Niederlande	MS Imaging Vortragend
Heidemann, Johannes	Heinrich-Pette-Institute, Leibniz Institute for Experimental Virology, Hamburg, Germany; Heinrich-Pette-Institut, Hamburg, Deutschland	Native Massespektrometrie Vortragend Poster Session Montag Abend
Heikaus, Laura	University Medical Center Hamburg-Eppendorf, Deutschland	Poster Session Montag Abend
Heikaus de Figueiredo, Laura	University Medical Center Hamburg Eppendorf, Deutschland	Proteine & Proteomics II Vortragend

Autor(en)	Organisation(en)	Session
Heiles, Sven	Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen	Ionisationsmethoden Lipide I Poster Session Montag Abend Vortragend
Heiling, Sven	Max Planck Institute for Chemical Ecology, Department for Molecular Ecology, Jena, Germany	Poster Session Montag Abend
Heimerl, Jule	Humboldt-Universität zu Berlin, Institut für Chemie, Deutschland	Poster Session Montag Abend
Heintze, Christoph	B-CUBE Center for Molecular Bioengineering, Dresden, Deutschland	Native Massespektrometrie
Helle, Niklas	Universität Kiel, Deutschland	Poster Session Montag Abend Vortragend
Hellwig, Nils	Goethe-University Frankfurt/Main, Deutschland; Institut für Physikalische und Theoretische Chemie, Goethe-Universität Frankfurt	Poster Session Montag Abend Poster Session Montag Abend Vortragend
Hempel, Ute	Institute of Physiological Chemistry, Faculty of Medicine Carl Gustav Carus, Technical University Dresden, Germany	Poster Session Montag Abend
Hendgen-Cotta, Ulrike B.	University Hospital Essen, Medical Faculty, West German Heart and Vascular Center, Department of Cardiology and Department of Angiology, Germany	Poster Session Montag Abend
Hendrikse, Jeanet	Netherlands Forensic Institute, Forensic Chemistry – Chemical Identification Analysis, 2497 GB The Hague, Netherlands	Analytische Anwendungen I
Henkel, Corinna	Bruker Daltonik GmbH, Bremen, Germany	Grundlagen und Instrumentelle Entwicklungen II
Henrion, André	Physikalisch-Technische-Bundesanstalt, Deutschland	Poster Session Montag Abend
Hense, Genia	Goethe Universität Frankfurt, Deutschland	Poster Session Montag Abend
Herfurth, Uta M.	Universität Leipzig, Fakultät für Chemie und Mineralogie, Germany	Analytische Anwendungen II
Hinz, Klaus Peter	Justus-Liebig Universität Giessen, Deutschland	Poster Session Montag Abend Poster Session Montag Abend Vortragend
Hirtz, Christophe	Laboratoire de Biochimie et Protéomique Clinique, Institut de Médecine Régénératrice et de Biothérapie, CHU de Montpellier - Hôpital St. Eloi, Montpellier, France	Poster Session Montag Abend
Hitzenberger, Jakob F.	Friedrich-Alexander-University Erlangen-Nürnberg, Germany	Gasphasenreaktionen & Fragmentierungen II Vortragend Gasphasenreaktionen & Fragmentierungen II
Hoehenwarter, Wolfgang	Proteome Analytics Research Group, Leibniz Institute of Plant Biochemistry	Poster Session Montag Abend
Hoffmann, Christian	Free Floater (Junior) Research Group Applied Synthetic Biology, Georg-August University Göttingen, Institute for Microbiology and Genetics, 37077 Göttingen, Germany	Poster Session Montag Abend
Hoffmann, Jan	University of Frankfurt, Deutschland	Native Massespektrometrie Poster Session Montag Abend
Hoffmann, Ralf	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig, Germany; Center for Biotechnology and Biomedicine, Universität Leipzig, Germany	Poster Session Montag Abend MS Analytik
Hoffmann, Waldemar	Freie Universität Berlin; Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin	Ionen Mobilität Poster Session Montag Abend Vortragend Grundlagen und Instrumentelle Entwicklungen II
Hofmann, Diana	Forschungszentrum Jülich, Deutschland	Poster Session Montag Abend Vortragend
Hofmann, Tommy	Interdisciplinary research center HALOmem, Martin Luther University Halle-Wittenberg, Kurt-Moses-Straße-3, 06120 Halle (Saale).; Helmholtz-Centre for Environmental research (UFZ), Department of Molecular Systems Biology, Leipzig, Germany; HALOmem, Halle (Saale), Germany	Lipide I Vortragend Poster Session Montag Abend

Autor(en)	Organisation(en)	Session
Holterhus, Paul-Martin	Universitätsklinikum Schleswig-Holstein, Deutschland	Klinische Diagnostik & Forensic
Hooton, Kevin	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster Session Montag Abend
Horner, Gerhard	Five Technologies GmbH, Frauenstrasse 22, 80469 Munich, Germany	Ionisationsmethoden Vortragend
Hoyes, John	Waters Corporation, Wilmslow, United Kingdom	Poster Session Montag Abend
Hübner, Florian	Institute of Food Chemistry, University of Münster, Germany	Poster Session Montag Abend
Hughes, Chris	Waters Corporation, Wilmslow, United Kingdom	Poster Session Montag Abend Poster Session Montag Abend
Humpf, Hans-Ulrich	Institute of Food Chemistry, University of Münster, Germany	Poster Session Montag Abend Poster Session Montag Abend
Hunger, Doreen	2Department of Microbiology, Institute of Biology, Martin-Luther University Halle-Wittenberg, Halle (Saale), Germany	Poster Session Montag Abend
Hunter, Christie	SCIEX, USA	Poster Session Montag Abend
Hutterli, Manuel	TOFWERK, Schweiz	Poster Session Montag Abend
Iacobucci, Claudio	UMR CNRS 6521, Université de Bretagne Occidentale, 6 Av.Le Gorgeu, 29200 Brest, France; Institute of Pharmacy, Martin-Luther University Halle-Wittenberg, Halle/Saale, Germany, Deutschland	Gasphasenreaktionen & Fragmentierungen I Vortragend
Ickert, Stefanie	Bundesanstalt für Materialforschung- und prüfung, Deutschland	Poster Session Montag Abend Vortragend
Ihling, Christian	Martin-Luther Universität Halle-Wittenberg, Deutschland; Martin-Luther-University Halle-Wittenberg, Institute of Pharmacy, Department of Pharmaceutical Chemistry and Bioanalytics, Germany; Institute of Pharmacy, Martin Luther University Halle-Wittenberg	Native Massespektrometrie Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend Proteine & Proteomics I Proteine & Proteomics II Vortragend
Ivanović-Burmacović, Ivana	Friedrich-Alexander-University Erlangen-Nürnberg, Deutschland	Poster Session Montag Abend
Jahn, Olaf	Max-Planck-Institut für experimentelle Medizin, Göttingen, Deutschland; Center for Nanoscale Microscopy and Molecular Physiology of the Brain, 37075 Göttingen, Germany	Native Massespektrometrie Poster Session Montag Abend Vortragend Proteine & Proteomics I
Jahnke, Siegfried	IBG-2 Pflanzenwissenschaften, Forschungszentrum Jülich, Deutschland	Poster Session Montag Abend
Jakimovska, Viktorija	Ss. Cyril and Methodius University of Skopje, Republic of Macedonia	Poster Session Montag Abend
Jakubowski, Norbert	Bundesanstalt für Materialforschung und -prüfung, Berlin	Poster Session Montag Abend
Janzik, Ingar	IBG-2 Pflanzenwissenschaften, Forschungszentrum Jülich, Deutschland	Poster Session Montag Abend
Jeck, Viola	Westfälische Wilhelms-Universität Münster, Deutschland	Poster Session Montag Abend Vortragend
Jeibmann, Astrid	University Hospital of Münster, Institute of Neuropathology, Münster, Germany	Bildgebende Massenspektrometrie
Jertz, Roland	Bruker Daltonik GmbH, Bremen, Germany	Grundlagen und Instrumentelle Entwicklungen II Poster Session Montag Abend
John, Harald	Bundeswehr Institute of Pharmacology and Toxicology	Poster Session Montag Abend Poster Session Montag Abend
Jones, Emrys	Waters Corporation, United Kingdom	Bildgebende Massenspektrometrie
Joseph, Shai R	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany, Deutschland	Proteine & Proteomics II
Josephs, Jonathan	Thermo Fisher Scientific, USA	Poster Session Montag Abend
Jurk, Kerstin	Center for Thrombosis and Hemostasis, Universitätsklinikum der Johannes	Proteine & Proteomics I

Autor(en)	Organisation(en)	Session
	Gutenberg-Universität Mainz, Mainz, Germany;	
Kade, Stephanie	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	Poster Session Montag Abend
Kadesch, Patrik	Justus-Liebig-Universität Gießen, Institut für Anorganische und Analytische Chemie	Analytische Anwendungen I Vortragend
Kaefer, Uwe	Cooperation Group ''Comprehensive Molecular Analytics", Helmholtz Zentrum Muenchen, Munich, GERMANY	Poster Session Montag Abend
Käfer, Uwe	Helmholtz Zentrum Muenchen, Neuherberg	Grundlagen und Instrumentelle Entwicklungen II Vortragend
Kaftan, Filip	Max Planck Institute for Chemical Ecology, Jena, Germany	Poster Session Montag Abend
Kaleja, Patrick	AG Systematische Proteomforschung & Bioanalytik, Institut für Experimentelle Medizin, Christian-Albrechts-Universität, Kiel; Klinik für Unfallchirurgie und Traumatologie, Experimentelle Unfallchirurgie, UKSH, Kiel	Poster Session Montag Abend Vortragend
Kalinowski, Jörn	Bielefeld University, Bielefeld, Deutschland	Poster Session Montag Abend
Kalkhof, Stefan	Helmholtz-Centre for Environmental research (UFZ), Department of Molecular Systems Biology, Leipzig, Germany; Coburg University, Department of Applied Sciences, Coburg, Germany	Poster Session Montag Abend Poster Session Montag Abend
Kanawati, Basem	Helmholtz Zentrum München, Deutschland	Grundlagen und Instrumentelle Entwicklungen II Vortragend
Kappert, Christin	Max Planck Institute for Biophysical Chemistry, Göttingen, Germany	Analytische Anwendungen II
Karaköse, Hande	Division of Bioanalytical Chemistry, Research Center Borstel, Germany; German Center for Infection Research, Clinical Tuberculosis Center, Borstel, Germany	Poster Session Montag Abend Vortragend
Karas, Michael	Goethe Universität, Frankfurt, Deutschland	Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend Proteine & Proteomics II
Karimi, Kudratullah	Goethe-University Frankfurt/Main, Deutschland	Poster Session Montag Abend Vortragend
Karst, Uwe	University of Münster, Institute of Inorganic and Analytical Chemistry, Münster, Germany; Westfälische Wilhelms-Universität Münster; Institut für Anorganische und Analytische Chemie, Universität Münster, Deutschland	Bildgebende Massenspektrometrie Bildgebende Massenspektrometrie Bildgebende Massenspektrometrie Metabolomics MS Analytik MS Analytik Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend
Kaspar-Schoenefeld, Stephanie	Bruker Daltonik GmbH, Deutschland	Poster Session Montag Abend
Kasuch, Sandra	Federal Criminal Police Office, Forensic Institute, 65193 Wiesbaden, Germany	Analytische Anwendungen I
Kaub, Johannes	Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Deutschland	Poster Session Montag Abend Vortragend
Kellner, Ina	Friedrich-Alexander-University Erlangen-Nürnberg, Deutschland	Poster Session Montag Abend Vortragend
Keppler, Bernhard K.	Universität Wien, Österreich	MS Analytik
Kessler, Nikolas	Bruker Daltonik GmbH, Deutschland	Poster Session Montag Abend
Kettling, Hans	University of Münster, Insitute for Hygiene, Münster, Germany; Interdisciplinary Center for Clinical Research (IZKF) Münster, Germany	Poster Session Montag Abend
Khalil, Saleh mahmud	Justus Liebig University Giessen, Institute of Inorganic and Analytical Chemistry	Bildgebende Massenspektrometrie Vortragend

Autor(en)	Organisation(en)	Session
Kiani, Parnian	University Medical Centre Hamburg-Eppendorf, Institute for Clinical Chemistry, Department for Mass Spectrometric Proteomics, Hamburg	Poster Session Montag Abend Vortragend
Kim, Ahyoung	Leibniz Institute of Plant Biochemistry, Department of Bioorganic Chemistry; Universität Leipzig, Faculty of Chemistry and Mineralogy	Poster Session Montag Abend Vortragend
Kiontke, Andreas	Universität Leipzig, Deutschland	Ionisationsmethoden Vortragend
Kipping, Marc	Waters GmbH, Eschborn, Deutschland	Poster Session Montag Abend Vortragend Poster Session Montag Abend Vortragend
Kirsch, Dieter	Federal Criminal Police Office, Forensic Institute, 65193 Wiesbaden, Germany	Analytische Anwendungen I
Kivala, Milan	Friedrich-Alexander-University Erlangen-Nürnberg, Germany	Gasphasenreaktionen & Fragmentierungen II
Klee, Sonja	TOFWERK, Schweiz	Poster Session Montag Abend Vortragend
Klein, Jonas	University Medical Center Hamburg-Eppendorf, Deutschland	Poster Session Montag Abend Vortragend
Kniese, Jasmin	Universität Bayreuth, Deutschland	Poster Session Montag Abend
Knochenmuss, Richard	Tofwerk, Uttigenstrasse 22, CH-3600 Thun, Switzerland	Ionen Mobilität
Koch, Annika	Institute for Hygiene, University of Münster, Robert-Koch-Str. 41, 48149 Münster, Germany	Poster Session Montag Abend
Koch, Annika	University of Münster, Institute of Hygiene, Biomedical Mass Spectrometry, Germany	Poster Session Montag Abend Vortragend
Koch, Arne	University of Leipzig, Germany	Poster Session Montag Abend
Koch, Winfried	Oil-Wärme-Institut GmbH, Herzogenrath, Deutschland	Poster Session Montag Abend
Koellensperger, Gunda	Universität Wien, Österreich	MS Analytik
Koenig, Stefan	Institute of Forensic Medicine, University of Bern	Poster Session Montag Abend
Köhler, Jörg	Markes International GmbH, Schleussnerstrasse 42, Frankfurt, Germany	Ionisationsmethoden
Köhler, Niklas	Division of Clinical Infectious Diseases, Research Center Borstel, Borstel, Germany; German Center for Infection Research, Clinical Tuberculosis Center, Borstel, Germany	Poster Session Montag Abend
Kokesch-Himmelreich, Julia	Universität Bayreuth, Deutschland	Poster Session Montag Abend
Kölbel, Knut	Universiteit Antwerpen, Belgien	Ionen Mobilität Vortragend
Kolter, Marlene	Georg-August-Universität Göttingen, Deutschland	Poster Session Montag Abend Vortragend
Komorowski, Lars	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	Poster Session Montag Abend
Kompauer, Mario	Justus Liebig University Giessen, Germany; Institut für Anorganische und Analytische Chemie; Justus-Liebig-Universität Gießen	Bildgebende Massenspektrometrie Vortragend Poster Session Montag Abend
Kondyli, Aikaterini	Max Planck Institut für Kohlenforschung, Germany	Poster Session Montag Abend Vortragend
Konietzny, Rebecca	Agilent Technologies, Waldbronn, Deutschland	Ionen Mobilität
König, Simone	WWU Münster	Proteine & Proteomics II
König, Vanessa	Hochschule Mannheim, Deutschland	Poster Session Montag Abend
Kopczynski, Dominik	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Germany	Lipide II MS-Informatik/Bioinformatik Vortragend
Kopicki, Janine	Heinrich-Pette-Institut, Hamburg, Deutschland	Poster Session Montag Abend Vortragend
Koschinski, Stefan	Markes International GmbH, Schleussnerstrasse 42, Frankfurt, Germany	Ionisationsmethoden
Köster, Claus	Bruker-Daltonik GmbH, Bremen	Poster Session Montag Abend
Koszinowski, Konrad	Georg-August-Universität Göttingen, Deutschland	Poster Session Montag Abend Poster Session Montag Abend Grundlagen und Instrumentelle

Autor(en)	Organisation(en)	Session
		Entwicklungen I Vortragend Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend
Kowol, Christian R.	Universität Wien, Österreich	MS Analytik
Kozlov, Ilya	University of Leipzig, Germany	Poster Session Montag Abend
Kraj, Agnieszka	ANTEC, Leyden	Poster Session Montag Abend
Krajewski, Matthias	Division of Bioanalytical Chemistry, Research Center Borstel, Parkallee 10, Borstel, Germany	Lipide I
Kramer, Katharina	Max Planck Institute for Plant Breeding Research, Köln, Germany	Analytische Anwendungen II
Kratochvil, Isabel	Helmholtz-Centre for Environmental research (UFZ), Department of Molecular Systems Biology, Leipzig, Germany	Poster Session Montag Abend Vortragend
Kraus, Johanna	Fort Collins Science Center, US Geological Survey, Fort Collins, USA	Bildgebende Massenspektrometrie
Krause, Eberhard	Leibniz Institut für Molekulare Pharmakologie, Deutschland	Poster Session Montag Abend Proteine & Proteomics I
Kreyenschmidt, Friedrich	Georg-August-Universität Göttingen, Deutschland	Grundlagen und Instrumentelle Entwicklungen I Poster Session Montag Abend Vortragend
Kriete, Claudia	Bruker Daltonik GmbH, Bremen, Germany	Grundlagen und Instrumentelle Entwicklungen II Poster Session Montag Abend
Kröger, Nils	B-CUBE Center for Molecular Bioengineering, Dresden, Deutschland; Department of Chemistry and Food Chemistry, Technische Universität Dresden, Deutschland	Native Massespektrometrie
Kröger, Sabrina	University of Münster, Institute of Inorganic and Analytical Chemistry, Münster, Germany	Bildgebende Massenspektrometrie Vortragend
Krösser, Dennis	University Medical Center Hamburg Eppendorf, Deutschland	Poster Session Montag Abend Poster Session Montag Abend Vortragend
Krüger, Sascha	Universität Kiel, Deutschland	Poster Session Montag Abend
Kruth, Claudia	Universität Rostock, Deutschland	Ionisationsmethoden
Kuballa, Juergen	GALAB Laboratories GmbH, Deutschland	MS-Informatik/Bioinformatik
Kuballa, Jürgen	GALAB Laboratories GmbH, Deutschland	Poster Session Montag Abend
Kuck, Dietmar	Department of Chemistry, Bielefeld University	Poster Session Montag Abend Vortragend Poster Session Montag Abend Vortragend
Kücklich, Marlen	Universität Leipzig, Deutschland	Poster Session Montag Abend
Kugler, Christian	LungenClinic Großhansdorf, Wöhrendamm 80, 22927 Großhansdorf.	Lipide II
Kühne, Stephan	Bruker Daltonik GmbH, Deutschland	Poster Session Montag Abend Vortragend Poster Session Montag Abend Vortragend
Kukačka, Zdeněk	Steinbeis Center for Biopolymer Analysis and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany	Poster Session Montag Abend
Kulkarni, Purva	Research Group Mass spectrometry/Proteomics, Max Planck Institute for Chemical Ecology; Chair for Bioinformatics, Friedrich Schiller University Jena; Max Planck Institute for Chemical Ecology, Jena, Germany	Grundlagen und Instrumentelle Entwicklungen I Metabolomics
Kulle, Alexandra	Universitätsklinikum Schleswig-Holstein, Deutschland	Klinische Diagnostik & Forensic Vortragend
Kumar, Mukesh	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany, Deutschland	Proteine & Proteomics II Vortragend
Kuo, Alex	Academia Sinica, School of Chemistry, Taipei, Taiwan	Poster Session Montag Abend
Kurulugama, Ruwan	Agilent Technologies, Santa Clara, USA	Ionen Mobilität
Kusch, Kathrin	Department of Neurogenetics, Max-Planck-Institute of Experimental Medicine, 37075 Göttingen, Germany	Poster Session Montag Abend

Autor(en)	Organisation(en)	Session
Kuzmich, Oleksandra	Humboldt Universität zu Berlin, Deutschland	Proteine & Proteomics I Vortragend
Kwiatkowski, Marcel	University Medical Center Groningen, Department of Pulmonary Diseases and Tuberculosis, Groningen, The Netherlands.; University of Groningen, Department of Analytical Biochemistry, The Netherlands.	Preisverleihung Wolfgang-Paul-Studienpreis Vortragend
Kwiatkowski, Marcel	Mass Spectrometric Proteomics, Department of Clinical Chemistry, University Medical Center Hamburg-Eppendorf, Hamburg, Germany.	Poster Session Montag Abend
Lang, Johannes	II physikalisches Insitut, Justus-Liebig-Universität Gießen, Deutschland	Poster Session Montag Abend
Lange, Christoph	Division of Clinical Infectious Diseases, Research Center Borstel, Borstel, Germany; German Center for Infection Research, Clinical Tuberculosis Center, Borstel, Germany; International Health/Infectious Diseases, University of Lübeck, Lübeck, Germany	Poster Session Montag Abend
Lange, Mike	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig; Center for Biotechnology and Biomedicine, Universität Leipzig, Germany	Lipide I
Lange, Tobias	University Medical Center Hamburg-Eppendorf, Deutschland	Poster Session Montag Abend
Langer, Julian	MPI for Biophysics, Frankfurt am Main, GERMANY	Poster Session Montag Abend
Langridge, James	Waters Corporation, Wilmslow, United Kingdom	Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend
Lebon, Alexandre	UMR CNRS 6521, Université de Bretagne Occidentale, 6 Av.Le Gorgeu, 29200 Brest, France	Gasphasenreaktionen & Fragmentierungen I
Lee, Hee-Jin	Humboldt-Universität zu Berlin, Deutschland	Poster Session Montag Abend
Lehmann, Sylvain	Laboratoire de Biochimie et Protéomique Clinique, Institut de Médecine Régénératrice et de Biothérapie, CHU de Montpellier - Hôpital St. Eloi, Montpellier, France	Poster Session Montag Abend
Lehmann, Wolf-Dieter	Biochemie-Zentrum Heidelberg, Deutschland; DKFZ Heidelberg; Deutsches Krebsforschungszentrum (DKFZ) Heidelberg	Lipide I Poster Session Montag Abend Vortragend
Leipert, Jan	AG Systematische Proteomforschung & Bioanalytik, Institut für Experimentelle Medizin, Christian-Albrechts-Universität zu Kiel, Kiel, Deutschland	Poster Session Montag Abend Vortragend
Lemesheva, Valeriia	St-Petersburg State University, Russia	Poster Session Montag Abend
Lemmnitzer, Katharina	University of Leipzig, Medical Faculty, Institute of Medical Physics and Biophysics	Ionen Mobilität Vortragend
Lenz, Thomas	caprotec bioanalytics GmbH	Proteine & Proteomics I
Leonhard, Peter	Merck KGaA, Frankfurter Str. 250, 64293 Darmstadt, Germany	Poster Session Montag Abend
Leveridge, Melanie	Departments of Platform Technology & Science, GlaxoSmithKline, Stevenage, UK	Poster Session Montag Abend
Lewin, Yannik	Goethe Universität, Frankfurt, Deutschland	Poster Session Montag Abend Vortragend
Li, Bin	Department of Chemistry, University of Illinois, 405 North Mathews Avenue, 61801 Urbana, Illinois, USA	Metabolomics
Li, Liang	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster Session Montag Abend
Li, Yan	Helmholtz Zentrum München, Deutschland	Grundlagen und Instrumentelle Entwicklungen II
Li, Zhendong	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster Session Montag Abend Poster Session Montag Abend
Lieblein, Tobias	Goethe-Universität Frankfurt, Deutschland	Native Massespektrometrie Vortragend

Autor(en)	Organisation(en)	Session
Liepold, Thomas	Proteomics Group, Max-Planck-Institute of Experimental Medicine, 37075 Göttingen, Germany	Poster Session Montag Abend
Linke, Dennis	Div. Systematic Proteome Research & Bioanalytics, Institute for Experimental Medicine, Kiel University, Germany	Poster Session Montag Abend
Linscheid, Michael	Humboldt-Universität zu Berlin	Poster Session Montag Abend Proteine & Proteomics I
Linscheid, Michael W.	Humboldt-Universität zu Berlin, Institut für Chemie, Deutschland	Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend
Lippert, Wayne	II physikalisches Insitut, Justus-Liebig-Universität Gießen, Deutschland	Poster Session Montag Abend
Liu, Fan	Universiteit Utrecht, The Netherlands	Poster Session Montag Abend
Lockhauserbäumer, Julia	Heinrich-Pette-Institute Leibniz Institute for Experimental Virology, Deutschland	Poster Session Montag Abend
Löhmannsröben, Hans-Gerd	University of Potsdam, Germany	Poster Session Montag Abend
Lopez, Javier	Bruker Espanola S.A., Madrid, Spanien	Poster Session Montag Abend
Lopez-Hilfiker, Felipe	TOFWERK, Schweiz; Paul Scherrer Institute (PSI), Villigen, Switzerland	Poster Session Montag Abend
Lorenz, Jana	1Department of Pharmaceutical Chemistry and Bioanalytics, Institute of Pharmacy, Martin-Luther University Halle-Wittenberg, Halle (Saale), Germany	Poster Session Montag Abend Vortragend
Lorenz, Yvonne	Universität Bonn, Deutschland	Poster Session Montag Abend Vortragend
Loroch, Stefan	Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund, Germany	Klinische Diagnostik & Forensic Vortragend Proteine & Proteomics I
Lotz, Florian	Justus-Liebig-Universität Gießen, Deutschland	Grundlagen und Instrumentelle Entwicklungen II Vortragend
Lubeck, Markus	Bruker Daltonik GmbH, Deutschland	Poster Session Montag Abend
Luckau, Luise	Physikalisch-Technische-Bundesanstalt, Deutschland	Poster Session Montag Abend Vortragend
Luetjohann, Jens	GALAB Laboratories GmbH, Deutschland	MS-Informatik/Bioinformatik Vortragend
Luginbühl, Marc	Institute of Forensic Medicine, University of Bern	Poster Session Montag Abend Vortragend
Lukasheva, Elena	Universität St. Petersburg, Lehrstuhl Biochemie, Russia	Analytische Anwendungen II
Luo, Ruoji	Max-Planck-Institut für Kohlenforschung, Deutschland	Poster Session Montag Abend Vortragend
Luo, Xian	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster Session Montag Abend
Lupu, Loredana	Steinbeis Center for Biopolymer Analysis and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany; Proteome Center, Institute of Immunology, University of Rostock, Rostock, Germany	Poster Session Montag Abend
Lützen, Elias	Westfählische Wilhelms-Universität Münster	Poster Session Montag Abend Vortragend
Maeser, Stefan	Steinbeis Center for Biopolymer Analysis and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany	Poster Session Montag Abend
Mairinger, Teresa	BOKU Wien, Österreich	Ionen Mobilität
Makowski, Marcus R.	Charité, Berlin	Poster Session Montag Abend
Mallagaray, Alvaro	Institute of Chemistry, University of Lübeck, Lübeck, Germany	Poster Session Montag Abend
Mannaa, Atef	Mass Spectrometric Proteomics, Department of Clinical Chemistry, University Medical Center Hamburg-Eppendorf, Hamburg, Germany.	Poster Session Montag Abend Vortragend
Manns, Annika	Leibniz Institut für Molekulare Pharmakologie, Deutschland	Poster Session Montag Abend Vortragend
Marcillo, Andrea	University of Leipzig, Germany	Poster Session Montag Abend Vortragend Poster Session Montag Abend

Autor(en)	Organisation(en)	Session
Marella, Chakravarthy	Research Center Borstel, Division of Bioanalytical Chemistry, Parkallee 1-40, D-23845 Borstel, Germany.	Lipide II
Marianski, Mateusz	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland	Grundlagen und Instrumentelle Entwicklungen II
Marshall, Peter	Departments of Platform Technology & Science, GlaxoSmithKline, Stevenage, UK	Poster Session Montag Abend
Martin, Diego	Bruker Espanola S.A., Madrid, Spanien	Poster Session Montag Abend
Massolini, Gabriella	Department of Drug Sciences, University of Pavia, Pavia, Italy	Poster Session Montag Abend
Matamoros, Manuel	Estación Experimental de Aula Dei, Consejo Superior de Investigaciones Científicas (CSIC), Department of Plant Nutrition	Poster Session Montag Abend
Matsubara, Shizue	IBG-2 Pflanzenwissenschaften, Forschungszentrum Jülich, Deutschland	Poster Session Montag Abend
Mattheij, Nadine J.	Department of Biochemistry, Cardiovascular Research Institute Maastricht, Maastricht University, The Netherlands;	Proteine & Proteomics I
Mävers, Stephan	Bruker Daltonik GmbH, Deutschland	Poster Session Montag Abend
May, Jody	Vanderbilt University, USA	Ionen Mobilität
Mazzone, Massimiliano	Laboratory of Molecular Oncology and Angiogenesis, Vesalius Research Center, Leuven, Belgium	Klinische Diagnostik & Forensic
McGregor, Laura	Markes International, Gwaun Elai Medi-Science Campus, Llantrisant, RCT, Wales, United Kingdom	Ionisationsmethoden
McLean, John	Vanderbilt University, USA	Ionen Mobilität
McLean, Lynn	Centre for Proteome Research, Institute of Integrative Biology, University of Liverpool, Liverpool, UK	Poster Session Montag Abend
Meckenstock, Rainer U.	Bio-film Center Universität Duisburg-Essen	Poster Session Montag Abend
Medvedev, Sergei	Department of Plant Physiology and Biochemistry, St. Petersburg State University	Poster Session Montag Abend Poster Session Montag Abend
Mehmood, Tahir	Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry, Germany	Poster Session Montag Abend
Meijers, Rob	European Molecular Biology Laboratory (EMBL), Hamburg, Germany	Native Massespektrometrie
Meiler, Jens	Vanderbilt University, Nashville, Tennessee, USA	Proteine & Proteomics I
Meinhardt, Ute	Friedrich-Alexander-University Erlangen-Nürnberg, Germany	Gasphasenreaktionen & Fragmentierungen II
Melzig, Matthias F.	Freie Universität Berlin, Institute of Pharmacy, Pharmaceutical Biology	Poster Session Montag Abend
Memboeuf, Antony	UMR CNRS 6521, Université de Bretagne Occidentale, 6 Av.Le Gorgeu, 29200 Brest, France	Gasphasenreaktionen & Fragmentierungen I
Menezes, Riya Christina	Max Planck Institute for Chemical Ecology, Jena, Germany	Metabolomics Vortragend
Mercanoglu, Baris	University Medical Center Hamburg Eppendorf, Deutschland	Poster Session Montag Abend
Meyer, Bernd	Uni Hamburg, Deutschland	Poster Session Montag Abend
Meyer, Nele	University of Bonn	Poster Session Montag Abend
Meyer, Stefanie	Friedrich Schiller University Jena, Deutschland	Analytische Anwendungen I
Meyer, Sven W.	Bruker Daltonik GmbH, Deutschland	Poster Session Montag Abend
Michaelis, Simon	caprotec bioanalytics GmbH	Proteine & Proteomics I
Michalski, Annette	Bruker Daltonik GmbH, Deutschland	Poster Session Montag Abend
Michalzik, Beate	Friedrich Schiller University Jena, Deutschland	Analytische Anwendungen I
Milentyev, Alexander	MPI-CBG, Dresden, Deutschland	Native Massespektrometrie Vortragend
Milkovska-Stamenova, Sanja	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig;	MS Analytik Vortragend

Autor(en)	Organisation(en)	Session
	Center for Biotechnology and Biomedicine, Universität Leipzig	
Miller, Dwayne	Max Planck Institute for the Structure and Dynamics of Matter	Poster Session Montag Abend Poster Session Montag Abend
Miller, Janet	Fort Collins Science Center, US Geological Survey, Fort Collins, USA	Bildgebende Massenspektrometrie
Miller, R. J. Dwayne	Max Planck Institute for the Structure and Dynamics of Matter, Atomically Resolved Dynamics Division, Luruper Chaussee 149, 22761 Hamburg, Germany.; Max Planck Institut für Struktur und Dynamik der Materie, Hamburg, Deutschland; Department of Chemistry and Physics, University of Toronto, Toronto, Canada	Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend
Milrud, Svetlana	Department of Plant Physiology and Biochemistry, St. Petersburg State University, Russia; Department of Biochemistry, St. Petersburg State University, Russia	Analytische Anwendungen II
Minameyer, Martin B.	Friedrich-Alexander-University Erlangen-Nürnberg, Germany	Poster Session Montag Abend Gasphasenreaktionen & Fragmentierungen II Vortragend
Mindukshev, Igor	Sechenov Institute of Evolutionary Physiology and Biochemistry, Russian Academy of Sciences, Saint Petersburg, Russia;	Proteine & Proteomics I
Mischnick, Petra	Technische Universität Braunschweig, Deutschland	Poster Session Montag Abend
Miske, Ramona	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	Poster Session Montag Abend
Mitrofanov, Elena	Christian-Albrechts-Universität, Deutschland	Poster Session Montag Abend Vortragend
Mnatsakanyan, Ruzanna	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig; Center for Biotechnology and Biomedicine, Universität Leipzig	MS Analytik
Möbius, Wiebke	Department of Neurogenetics, Max-Planck-Institute of Experimental Medicine, 37075 Göttingen, Germany; Center for Nanoscale Microscopy and Molecular Physiology of the Brain, 37075 Göttingen, Germany	Poster Session Montag Abend
Mock, Hans-Peter	IPK-Gatersleben, Deutschland	Poster Session Montag Abend
Moise, Adrian	Department of Chemistry, University of Konstanz, Konstanz, Germany	Poster Session Montag Abend
Mokhtar, Mohamed	Christian-Albrechts-Universität zu Kiel, Deutschland	Poster Session Montag Abend
Möller, Manfred	Uniklinik der RWTH Aachen, Deutschland	Poster Session Montag Abend
Möller, Stephanie	Biomaterials Department, INNOVENT e.V., Jena, Germany	Poster Session Montag Abend
Mordehai, Alex	Agilent Technologies, Santa Clara, USA	Ionen Mobilität
Morgner, Nina	Goethe-Universität Frankfurt, Deutschland; Institut für Physikalische und Theoretische Chemie, Goethe-Universität Frankfurt	Native Massespektrometrie Native Massespektrometrie Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend
Mormann, Michael	Institut für Hygiene, Universität Münster, Deutschland	Poster Session Montag Abend Poster Session Montag Abend
Morrice, Nick	SCIEX, UK	Poster Session Montag Abend
Mucek, Katharina	Bioanalytical Mass Spectrometry, Max Planck Institute for Biophysical Chemistry, Göttingen, Germany	Poster Session Montag Abend Vortragend
Mucha, Eike	Freie Universität Berlin, Deutschland; Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland	Grundlagen und Instrumentelle Entwicklungen II

Autor(en)	Organisation(en)	Session
Mueller, Jennifer-Christin	Institute of Inorganic and Analytical Chemistry, University of Muenster, Corrensstr. 28/30, 48149 Muenster, Germany	Poster Session Montag Abend Vortragend
Mueller, Max A.	Justus Liebig University Giessen, Germany	Bildgebende Massenspektrometrie
Mülbaier, Marcel	Cellzome GmbH, Heidelberg	Proteine & Proteomics I
Müller, Julia	Pathology of the University Hospital of Lübeck and the Research Center Borstel, Clinical and Experimental Pathology, 23538 Lübeck and 23845 Borstel, Germany.	Lipide II
Müller, Katrin	Cellzome GmbH, Heidelberg	Proteine & Proteomics I
Müller, Mathias	Thermo Fisher Scientific, Bremen, Germany	Poster Session Montag Abend Vortragend
Müller, Miriam J.	Universität des Saarlandes, Saarbrücken, Deutschland; Saarland University, Deutschland	Klinische Diagnostik & Forensic Metabolomics Vortragend
Müller, Volker	Johann Wolfgang Goethe-Universität, Deutschland	Poster Session Montag Abend
Mung, Dorothea	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster Session Montag Abend
Muñoz-Fontela, Cesar	Heinrich-Pette-Institut, Hamburg, Deutschland	Poster Session Montag Abend
Münster-Müller, Sascha	Bundeskriminalamt Wiesbaden	Poster Session Montag Abend
Muskat, Tassilo	Christian-Albrechts-Universität, Deutschland	Poster Session Montag Abend
Näthe, Kerstin	Friedrich Schiller University Jena, Deutschland	Analytische Anwendungen I
Neese, Stephan	Justus-Liebig-Univeristät Gießen, Deutschland	Poster Session Montag Abend
Neubauer, Lisa	Institute of Plant Biology and Biotechnology, University of Münster, Germany	Poster Session Montag Abend
Neugebauer, Thomas	Friedrich-Alexander-University Erlangen-Nürnberg, Deutschland	Poster Session Montag Abend Vortragend
Neumann, Anika	Joint Mass Spectrometry Centre / Chair of Analytical Chemistry, University of Rostock, 18059 Rostock, Germany	Analytische Anwendungen I Poster Session Montag Abend Vortragend
Neumann, Heinz	Free Floater (Junior) Research Group Applied Synthetic Biology, Georg-August University Göttingen, Institute for Microbiology and Genetics, 37077 Göttingen, Germany	Poster Session Montag Abend
Neupärtl, Moritz	Goethe-Universität-Frankfurt	Proteine & Proteomics II
Neuweger, Heiko	Bruker Daltonik GmbH, Deutschland	Poster Session Montag Abend Poster Session Montag Abend
Neuwohner, Andrea	IBG-2 Pflanzenwissenschaften, Forschungszentrum Jülich, Deutschland	Poster Session Montag Abend
Nguyen, Minh	ISAS, Deutschland	Proteine & Proteomics II
Ni, Zhixu	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig; Center for Biotechnology and Biomedicine, Universität Leipzig, Germany	Lipide I
NicDaeid, Niamh	University of Dundee, CAHID, School of Science and Engineering, Dundee, DD15EH, Scotland	Analytische Anwendungen I
Niehoff, Ann-Christin	University of Münster, Institute of Inorganic and Analytical Chemistry, Münster, Germany	Bildgebende Massenspektrometrie
Nikolaev, Eugene N.	Institute for Energy Problems of Chemical Physics, Russian Academy of Sciences, Moscow, Russia	Poster Session Montag Abend Grundlagen und Instrumentelle Entwicklungen II
O'Hair, Richard	University of Melbourne, Australia	Poster Session Montag Abend
Oefner, Peter J.	University of Regensburg, Institute of Functional Genomics, Regensburg, Deutschland	Poster Session Montag Abend
Opuni, Kwabena F.M.	Proteome Center Rostock, Deutschland	Ionen Mobilität
Oster, M.	2Joint Mass Spectrometry Centre Helmholtz-Zentrum München,	Poster Session Montag Abend

Autor(en)	Organisation(en)	Session
	Comprehensive Molecular Analytics (CMA), Neuherberg, Germany	
Othman, Alaa	University of Lübeck, Germany	Metabolomics
O'Hair, Richard A. J.	The University of Melbourne, Australia	Massenspektrometrische Entwicklungen Vortragend
Pagel, Kevin	Freie Universität Berlin, Deutschland; Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland	Grundlagen und Instrumentelle Entwicklungen II Vortragend Ionen Mobilität Native Massespektrometrie Poster Session Montag Abend
Papan, Cyrus	SCIEX GmbH, Darmstadt, GERMANY	Poster Session Montag Abend Vortragend
Parchomyk, Tobias	Georg-August-Universität Göttingen, Deutschland	Poster Session Montag Abend Vortragend
Passig, Johannes	Universität Rostock, Deutschland; Joint Mass Spectrometry Centre University of Rostock, Chair of Analytical Chemistry, Rostock, Germany	Ionisationsmethoden Poster Session Montag Abend Vortragend
Paudel, Gagan	Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry (Halle/Saale); Faculty of Chemistry and Mineralogy, Universität Leipzig	Analytische Anwendungen II
Paudyal, Bhesh Raj	Department of Cellular Microbiology, Research Center Borstel, Parkallee 22, Borstel, Germany	Lipide I
Peetz, Oliver	University of Frankfurt, Deutschland	Native Massespektrometrie Vortragend
Peng, Bing	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Germany	Lipide II Vortragend
Penkert, Martin	Leibniz-Institut für molekulare Pharmakologie (FMP), Deutschland; Humboldt-Universität zu Berlin	Proteine & Proteomics I Vortragend
Penner, Alexander	Justus-Liebig-Univeristät Gießen, Deutschland	Poster Session Montag Abend
Perez, Cesar	Bruker Espanola S.A., Madrid, Spanien	Poster Session Montag Abend
Persicke, Marcus	Bielefeld University, Bielefeld, Deutschland	Poster Session Montag Abend
Peters, Thomas	Institute of Chemistry, University of Lübeck, Lübeck, Germany	Poster Session Montag Abend
Pietschke, Cleo	Zoologisches Institut, Uni Kiel	Poster Session Montag Abend
Pikhtelev, Alexander	Institute of Energy Problems of Chemical Physics, Russian Academy of Sciences, Russia	Poster Session Montag Abend
Piotrowski, Christine	Martin-Luther-Universität Halle-Wittenberg, Deutschland	Proteine & Proteomics I Vortragend
Planitz, Peter	Agilent Technologies, Waldbronn, Germany	MS Analytik
Plaß, Wolfgang R.	II physikalisches Insitut, Justus-Liebig-Universität Gießen, Deutschland; GSI Darmstadt, Deutschland	Poster Session Montag Abend
Poeckel, Daniel	Cellzome GmbH, Heidelberg	Proteine & Proteomics I
Pogan, Ronja	Heinrich-Pette-Institute Leibniz Institute for Experimental Virology, Deutschland	Poster Session Montag Abend Vortragend
Pohlentz, Gottfried	Institut für Hygiene, Universität Münster, Deutschland	Poster Session Montag Abend Vortragend
Popkova, Yulia	Leipzig University, Faculty of Medicine, Institute for Medical Physics and Biophysics, Germany	Grundlagen und Instrumentelle Entwicklungen I Vortragend
Pospilova, Veronika	Paul Scherrer Institute (PSI), Villigen, Switzerland	Poster Session Montag Abend
Potthoff, Alexander	Institute for Hygiene, University of Münster, Robert-Koch-Str. 41, 48149 Münster, Germany	Poster Session Montag Abend Vortragend
Pötz, Oliver	Natural and Medical Sciences Institute at the University of Tübingen, Tübingen, Germany;	Proteine & Proteomics I
Poulsen, Nicole	B-CUBE Center for Molecular Bioengineering, Dresden, Deutschland	Native Massespektrometrie
Prasse, Daniela	Institute for General Microbiology, Kiel University, Germany	Poster Session Montag Abend

Autor(en)	Organisation(en)	Session
Probst, Christian	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	Poster Session Montag Abend
Przybylski, Michael	Steinbeis Center for Biopolymer Analysis and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany	Poster Session Montag Abend Poster Session Montag Abend
Pütz, Michael	Bundeskriminalamt Wiesbaden	Poster Session Montag Abend
Quack, Thomas	Justus-Liebig-Universität Gießen, Institut für Parasitologie	Analytische Anwendungen I
Rabe, Klaus F.	LungenClinic Großhansdorf, Wöhrendamm 80, 22927 Großhansdorf.; Airway Research Center North, German Center for Lung Research, Wöhrendamm 80, 22927 Großhansdorf, Germany	Lipide II
Raja, Erum	Thermo Fisher Scientific, Rockford, IL, USA	Poster Session Montag Abend
Raupers, Björn	Universität Kiel, Deutschland	Poster Session Montag Abend Vortragend
Rehkamp, Anne	Martin-Luther-University Halle-Wittenberg, Institute of Pharmacy, Department of Pharmaceutical Chemistry and Bioanalytics, Germany	Poster Session Montag Abend Vortragend
Reinert, Thorben	Christian-Albrechts-Universität zu Kiel, Deutschland	Poster Session Montag Abend Vortragend
Renné, Thomas	University Medical Center Hamburg Eppendorf, Deutschland	Proteine & Proteomics II
Rennie, Emma	Agilent Technologies, Santa Clara, USA	Ionen Mobilität
Reuter, Jörn Hendrik	Research and Development, Beiersdorf AG, Hamburg	Poster Session Montag Abend
Richardson, Keith	Waters Corporation, Wilmslow, United Kingdom	Poster Session Montag Abend Poster Session Montag Abend
Riebe, Daniel	University of Potsdam, Germany	Poster Session Montag Abend
Riedel, Jens	Bundesanstalt für Materialforschung- und prüfung, Deutschland	Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend
Riemer, Thomas	University of Leipzig, Medical Faculty, Institute of Medical Physics and Biophysics	Ionen Mobilität
Rinaldi, Francesca	Department of Drug Sciences, University of Pavia, Pavia, Italy	Poster Session Montag Abend Vortragend
Rissanen, Kari	Department of Chemistry, NanoScience Center, University of Jyvaskyla, Finnland	Ionen Mobilität
Robertson, Wesley D.	Max Planck Institut für Struktur und Dynamik der Materie, Hamburg, Deutschland	Poster Session Montag Abend Poster Session Montag Abend
Röcken, Christoph	Institute of Pathology, Christian-Albrechts-Universität, Kiel, Germany	Klinische Diagnostik & Forensic
Roeck, Walter	Bruker BioSpin AG, Fällanden, Switzerland	Grundlagen und Instrumentelle Entwicklungen II
Rohn, Sascha	Universität Hamburg, Grindelallee 117, Hamburg; Universität Hamburg, Deutschland	Poster Session Montag Abend Poster Session Montag Abend
Rohner, Urs	TOFWERK, Switzerland	Poster Session Montag Abend Vortragend
Romanovskaya, Ekaterina	Department of Biochemistry, St. Petersburg State University, Russia	Poster Session Montag Abend
Römpp, Andreas	Chair of Bioanalytical Sciences and Food Analysis, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth, Germany; Department of Food Analysis, University of Bayreuth, E.-C.-Baumann-Str. 20, 95326 Kulmbach, Bayreuth, Germany; Universität Bayreuth, Deutschland	Bildgebende Massenspektrometrie Vortragend Metabolomics Poster Session Montag Abend Poster Session Montag Abend
Roth, Alexander	Hochschule Mannheim, Deutschland	Poster Session Montag Abend Vortragend
Rüger, Christopher Paul	University of Rostock, Rostock; Joint Mass Spectrometry Centre / Chair of Analytical Chemistry, University of Rostock, 18059 Rostock, Germany	Grundlagen und Instrumentelle Entwicklungen II Poster Session Montag Abend Analytische Anwendungen I Vortragend
Rühl, Michael	Goethe-Universität Frankfurt am Main, Deutschland	Poster Session Montag Abend Vortragend Poster Session Montag Abend

Autor(en)	Organisation(en)	Session
Rurack, Knut	Bundesanstalt für Materialforschung und -prüfung	Poster Session Montag Abend
Rutjens, Sofie	Laboratory of Toxicology, University of Ghent	Poster Session Montag Abend
Rychlik, Michael	Technische Universität Münschen, Lehrstuhl für Analytische Lebensmittelchemie	Poster Session Montag Abend
Saluz, Hans Peter	Department Cell and Molecular Biology, Leibniz Institute for Natural Product Research and Infection Biology	Grundlagen und Instrumentelle Entwicklungen I
Sanchez-Carballo, Patricia	Division of Clinical Infectious Diseases, Research Center Borstel, Borstel, Germany; German Center for Infection Research, Clinical Tuberculosis Center, Borstel, Germany	Poster Session Montag Abend
Satilmis, Ilker	Max-Planck-Institut für Kohlenforschung, Deutschland	Poster Session Montag Abend Vortragend
Sauerland, Volker	Bruker Daltonik GmbH, Germany	Poster Session Montag Abend
Savitski, Mikhail M.	Cellzome GmbH, Heidelberg; EMBL, Heidelberg	Proteine & Proteomics I
Sawers, Gary	2Department of Microbiology, Institute of Biology, Martin-Luther University Halle-Wittenberg, Halle (Saale), Germany	Poster Session Montag Abend
Schachel, Tilo D.	Westfälische Wilhelms-Universität Münster, Deutschland	Poster Session Montag Abend Vortragend
Schade, Julian	Joint Mass Spectrometry Centre University of Rostock, Chair of Analytical Chemistry, Rostock, Germany	Poster Session Montag Abend
Schäfer, Frank	Federal Criminal Police Office, Forensic Institute, 65193 Wiesbaden, Germany	Analytische Anwendungen I
Schäfer, Mathias	Universität zu Köln, Deutschland; Institute for Organic Chemistry, Department of Chemistry, University of Cologne	Poster Session Montag Abend Proteine & Proteomics II Gasphasenreaktionen & Fragmentierungen II
Schäfer, Mathias	Institute of Organic Chemistry, University of Cologne, Greinstraße 4, 50939 Köln, Germany	Lipide I
Schaible, Ulrich E.	Department of Cellular Microbiology, Research Center Borstel, Parkallee 22, Borstel, Germany	Lipide I
Schalley, Christoph A.	Freie Universität Berlin	Ionen Mobilität
Scharf, Madeleine	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	Poster Session Montag Abend
Scharrenbroch, Lisa	Federal Criminal Police Office, Forensic Institute, 65193 Wiesbaden, Germany; University of Dundee, CAHID, School of Science and Engineering, Dundee, DD15EH, Scotland	Analytische Anwendungen I Vortragend
Schatz, Jürgen	Friedrich-Alexander-University Erlangen-Nürnberg, Germany	Gasphasenreaktionen & Fragmentierungen II
Scheeren, Simon Gereon	Westfälische Wilhelms-Universität Münster, Deutschland	Metabolomics Vortragend
Scheffler, Kai	Thermo Fisher Scientific, Deutschland	Poster Session Montag Abend Poster Session Montag Abend
Scheidegger, Oliver	Hoffmann la Roche AG, Schweiz	Poster Session Montag Abend
Scheidenberger, Christoph	II physikalisches Insitut, Justus-Liebig-Universität Gießen, Deutschland; GSI Darmstadt, Deutschland	Poster Session Montag Abend
Scheier, Rico	Universität Bayreuth, Deutschland	Poster Session Montag Abend
Schelhaas, Mario	Institute of Molecular Virology & Institute of Medical Biochemistry Münster, WW University of Münster, Germany	Poster Session Montag Abend
Schenk, Regina	Humboldt-Universität zu Berlin, Albrecht Daniel Thaer-Institute for Crop Science	Poster Session Montag Abend
Schiller, Jürgen	Leipzig University, Faculty of Medicine, Institute for Medical Physics and Biophysics, Germany	Grundlagen und Instrumentelle Entwicklungen I Ionen Mobilität

Autor(en)	Organisation(en)	Session
Schilyaev, Nikita	Universität St. Petersburg, Lehrstuhl Biochemie, Russia	Analytische Anwendungen II
Schlichting, Rita	Helmholtz-Centre for Environmental research (UFZ), Department of Cell Toxicology, Leipzig, Germany	Poster Session Montag Abend
Schlüter, Hartmut	University Medical Center Hamburg-Eppendorf, Deutschland	MS-Informatik/Bioinformatik Poster Session Montag Abend
Schlüter, Hartmut	Universitätsklinikum Hamburg-Eppendorf, Germany; University Medical Center Hamburg-Eppendorf, Deutschland; Mass Spectrometric Proteomics, Department of Clinical Chemistry, University Medical Center Hamburg-Eppendorf, Hamburg, Germany.; University Medical Centre Hamburg-Eppendorf, Institute of Clinical Chemistry, Department for Mass Spectrometric Proteomics, Hamburg Germany	Analytische Anwendungen II Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend Proteine & Proteomics II
Schmid, Robin	Institute of Food Chemistry, University of Münster, Germany; Institute of Inorganic and Analytical Chemistry, University of Münster, Germany	Poster Session Montag Abend Vortragend
Schmidt, Carla	Interdisciplinary research center HALOmem, Martin Luther University Halle-Wittenberg, Kurt-Moses-Straße-3, 06120 Halle (Saale).	Poster Session Montag Abend Proteine & Proteomics I Vortragend Lipide I
Schmidt, Charlie	PerkinElmer LAS (Germany) GmbH, Deutschland	Poster Session Montag Abend
Schmidt, Heinar	Universität Bayreuth, Deutschland	Poster Session Montag Abend
Schmidt, Johannes R.	Department for Molecular Systems Biology, Helmholtz Centre for Environmental Research – UFZ, Leipzig, Germany	Poster Session Montag Abend Vortragend
Schmidt, Rico	Institute of Pharmacy, Martin-Luther Universität Halle-Wittenberg	Analytische Anwendungen II Poster Session Montag Abend
Schmidt, Travis	Fort Collins Science Center, US Geological Survey, Fort Collins, USA	Bildgebende Massenspektrometrie
Schmit, Pierre-Olivier	Bruker Daltonik GmbH, Deutschland; Bruker Daltonique Wissembourg, France	Poster Session Montag Abend Poster Session Montag Abend
Schmitt-Kopplin, Philippe	Helmholtz Zentrum München, Deutschland; Technische Universität München	Grundlagen und Instrumentelle Entwicklungen II
Schmitz, Ruth A.	Institute for General Microbiology, Kiel University, Germany	Poster Session Montag Abend
Schnapp, Andreas	Institute for Hygiene, Biomedical Mass Spectrometry, University of Münster, Germany; Institute for Hygiene, University of Münster, Robert-Koch-Str. 41, 48149 Münster, Germany	Poster Session Montag Abend Poster Session Montag Abend
Schöllkopf, Wieland	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland	Grundlagen und Instrumentelle Entwicklungen II
Scholz, Verena	Research Center Borstel, Division of Bioanalytical Chemistry, Parkallee 1-40, D-23845 Borstel, Germany.	Lipide II
Schönborn, Stefan	Goethe-Universität Frankfurt am Main, Deutschland	Poster Session Montag Abend
Schrader, Wolfgang	Max-Planck-Institut für Kohlenforschung, Deutschland	Grundlagen und Instrumentelle Entwicklungen II Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend Gasphasenreaktionen & Fragmentierungen I Poster Session Montag Abend
Schriewer, Alexander	WWU Münster, Deutschland	Metabolomics Vortragend
Schubert, Ulrich S.	Friedrich Schiller University Jena, Deutschland	Analytische Anwendungen I
Schuhmann, Kai	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Deutschland	Analytische Anwendungen II Vortragend Lipide I

Autor(en)	Organisation(en)	Session
Schulz, Sabine	Justus-Liebig-Universität Gießen, Deutschland	Grundlagen und Instrumentelle Entwicklungen II Poster Session Montag Abend
Schümann, Michael	Leibniz Institut für Molekulare Pharmakologie, Deutschland	Poster Session Montag Abend Proteine & Proteomics I
Schütze, Johannes	IPK-Gatersleben, Deutschland	Poster Session Montag Abend Vortragend
Schwaiger-Hufnagel, Ulrike	Bruker Daltonik GmbH, Bremen, Germany	Poster Session Montag Abend
Schwemer, Theo	Joint Mass Spectrometry Centre / Chair of Analytical Chemistry, University of Rostock, 18059 Rostock, Germany; HICE - Helmholtz Virtual of Complex Molecular Systems in Environmental Health – Aerosols and Health, www.hice-vi.eu	Analytische Anwendungen I
Schwudke, Dominik	Division of Bioanalytical Chemistry, Research Center Borstel, Parkallee 10, Borstel, Germany; Airway Research Center North, German Center for Lung Research, Wöhrendamm 80, 22927 Großhansdorf, Germany; German Center for Infection Research, Clinical Tuberculosis Center, Borstel, Germany; Research Centre Borstel, Department of Bioanalytical Chemistry, Borstel Germany	Lipide I Lipide II Poster Session Montag Abend Poster Session Montag Abend
Seeberger, Peter	Freie Universität Berlin, Deutschland; Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Potsdam, Deutschland	Grundlagen und Instrumentelle Entwicklungen II
Seulen, Sarah	Christian-Albrechts-Universität zu Kiel, Deutschland	Gasphasenreaktionen & Fragmentierungen II Vortragend
Shadyro, Oleg	Belarusian State University, Department of Chemistry, Leningradskaya 14, 220006, Minsk, Belarus	Lipide II
Shema, Gerta	ISAS, Deutschland	Proteine & Proteomics II
Shevchenko, Andrej	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Deutschland; MPI-CBG, Dresden, Deutschland	Analytische Anwendungen II Biologische Massenspektrometrie Vortragend Lipide I Native Massespektrometrie Poster Session Montag Abend Proteine & Proteomics II
Shevchenko, Anna	MPI of Cell Biology and Genetics, Dresden, Germany	Poster Session Montag Abend
Shilyaev, Nikita	Department of Biochemistry, St. Petersburg State University, Russia	Analytische Anwendungen II
Sickmann, Albert	Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund, Germany; Department of Chemistry, College of Physical Sciences, University of Aberdeen, United Kingdom; Medizinisches Proteom Center, Ruhr Universität Bochum, Germany	Klinische Diagnostik & Forensic Proteine & Proteomics I Vortragend
Siegert, Markus	Department of Chemistry, Humboldt Universität zu Berlin, Berlin, Germany	Poster Session Montag Abend Vortragend
Siemers, Adrian	Analytik Jena AG, Jena, Germany	Poster Session Montag Abend
Simon, Fabian	Hochschule Mannheim, Deutschland	Poster Session Montag Abend
Sinz, Andrea	Institute of Pharmacy, Martin-Luther Universität Halle-Wittenberg; Martin-Luther-University Halle-Wittenberg, Institute of Pharmacy, Department of Pharmaceutical Chemistry and Bioanalytics, Germany; 1Department of Pharmaceutical Chemistry and Bioanalytics, Institute of Pharmacy, Martin-Luther University Halle-Wittenberg, Halle (Saale), Germany	Analytische Anwendungen II Gasphasenreaktionen & Fragmentierungen II Native Massespektrometrie Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend Proteine & Proteomics I Proteine & Proteomics II
Sklorz, Martin	Joint Mass Spectrometry Centre / Chair of Analytical Chemistry, University of Rostock,	Analytische Anwendungen I Ionisationsmethoden

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	18059 Rostock, Germany; Universität Rostock, Deutschland	Poster Session Montag Abend Poster Session Montag Abend
Slowik, Jay	Paul Scherrer Institute (PSI), Villigen, Switzerland	Poster Session Montag Abend
Smolikova, Galina	Department of Plant Physiology and Biochemistry, St. Petersburg State University, Russia	Analytische Anwendungen II Poster Session Montag Abend Poster Session Montag Abend
Soboleva, Alena	Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry, Germany; Department of Biochemistry, St. Petersburg State University, Russia	Poster Session Montag Abend
Sobott, Frank	Universiteit Antwerpen, Belgien	Ionen Mobilität
Solari, Fiorella A.	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Deutschland	Proteine & Proteomics I
Soltwisch, Jens	Institute for Hygiene, Biomedical Mass Spectrometry, University of Münster, Germany; Interdisciplinary Center for Clinical Research (IZKF), University of Münster, Germany; University of Münster, Insitute for Hygiene, Münster, Germany; Institute for Hygiene, University of Münster, Robert-Koch-Str. 41, 48149 Münster, Germany	Grundlagen und Instrumentelle Entwicklungen I Poster Session Montag Abend Poster Session Montag Abend Vortragend Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend
Spengler, Bernhard	Justus-Liebig-Universität Gießen, Institut für Anorganische und Analytische Chemie; Justus Liebig University, Gießen, Deutschland; Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen	Analytische Anwendungen I Analytische Anwendungen I Bildgebende Massenspektrometrie Bildgebende Massenspektrometrie Grundlagen und Instrumentelle Entwicklungen II Ionisationsmethoden Lipide I Metabolomics Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend
Sperling, Michael	Westfälische Wilhelms-Universität Münster; European Virtual Institute for Speciation Analysis; Institute of Inorganic and Analytical Chemistry, University of Münster, Münster, Germany	Bildgebende Massenspektrometrie MS Analytik
Spiteller, Peter	Universität Bremen, Deutschland	Poster Session Montag Abend
Springer, Andreas	Freie Universität Berlin, Institute of Chemistry and Biochemistry, Core Facility BioSupraMol	Poster Session Montag Abend
Stafford, George	Agilent Technologies, Santa Clara, USA	Ionen Mobilität
Stark, Tina	Goethe-Universität Frankfurt, Deutschland	Native Massespektrometrie
Steffen, Bernhard	Forschungszentrum Jülich, Deutschland	Poster Session Montag Abend
Steffen, Pascal	University Medical Center Hamburg-Eppendorf, Deutschland	MS-Informatik/Bioinformatik Vortragend Poster Session Montag Abend Poster Session Montag Abend
Stephanowitz, Heike	Leibniz Institut für Molekulare Pharmakologie, Deutschland	Poster Session Montag Abend
Stöcker, Winfried	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	Poster Session Montag Abend
Stokes, Caroline	Universitätsklinikum des Saarlandes, Homburg, Deutschland	Klinische Diagnostik & Forensic
Stow, Sarah	Vanderbilt University, USA	Ionen Mobilität
Streibel, Thorsten	Universität Rostock, Deutschland; Helmholtz-Zentrum München,Deutschland	Poster Session Montag Abend
Striegel, Lisa	Technische Universität Münschen, Lehrstuhl für Analytische Lebensmittelchemie	Poster Session Montag Abend
Struwe, Weston B.	Oxford Glycobiology Institute, Universität Oxford, Oxford, UK	Grundlagen und Instrumentelle Entwicklungen II

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Stummer, Walter	University Hospital of Münster, Department of Neurosurgery, Münster, Germany	Bildgebende Massenspektrometrie
Sturm, Patrick	TOFWERK, Switzerland	Poster Session Montag Abend
Stützer, Alexandra	Max Planck Institute for Biophysical Chemistry, Göttingen, Germany	Analytische Anwendungen II Vortragend Poster Session Montag Abend
Suckau, Detlev	Bruker Daltonik GmbH, Deutschland	Metabolomics Vortragend
Süß, Rosmarie	University of Leipzig, Medical Faculty, Institute of Medical Physics and Biophysics	Ionen Mobilität
Sutton, Jennifer	Thermo Fisher Scientific, USA	Poster Session Montag Abend
Svatoš, Aleš	Research Group Mass spectrometry/Proteomics, Max Planck Institute for Chemical Ecology; Max Planck Institute for Chemical Ecology, Jena, Germany; Institute of Organic Chemistry and Biochemistry, AS CR, Prague, Czech Republic	Grundlagen und Instrumentelle Entwicklungen I Metabolomics Poster Session Montag Abend
Szesny, Matthias	Bruker Daltonik GmbH, Deutschland	Metabolomics Vortragend Poster Session Montag Abend Vortragend Poster Session Montag Abend Vortragend Poster Session Montag Abend Vortragend
Tampé, Robert	Johann Wolfgang Goethe-Universität, Deutschland	Poster Session Montag Abend
Tanner, Martin	TOFWERK, Switzerland	Poster Session Montag Abend
Tarakhovskaya, Elena	Department of Plant Physiology and Biochemistry, St. Petersburg State University, Russia; St-Petersburg State University, Russia	Analytische Anwendungen II Poster Session Montag Abend Vortragend
Tatlay, Jaspaul	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster Session Montag Abend
Teegen, Bianca	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	Poster Session Montag Abend
Temporini, Caterina	Department of Drug Sciences, University of Pavia, Pavia, Italy	Poster Session Montag Abend
Tengattini, Sara	Department of Drug Sciences, University of Pavia, Pavia, Italy	Poster Session Montag Abend
Thiele, Björn	IBG-2 Pflanzenwissenschaften, Forschungszentrum Jülich, Deutschland	Poster Session Montag Abend Vortragend
Thiermann, Horst	Bundeswehr Institute of Pharmacology and Toxicology	Poster Session Montag Abend Poster Session Montag Abend
Thiesen, Hans-Jürgen	Institute of Immunology, University of Rostock, Germany	Ionen Mobilität
Tholey, Andreas	Systematic Proteome Research & Bioanalytics, Institute of Experimental Medicine, Christian-Albrechts-Universität, Kiel, Germany; Christian-Albrechts-Universität zu Kiel, Deutschland; Institut für Experimentelle Medizin, Uni Kiel	Klinische Diagnostik & Forensic Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend
Thomas, Daniel A.	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland	Grundlagen und Instrumentelle Entwicklungen II
Thomas, Henrik	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Deutschland	Analytische Anwendungen II Poster Session Montag Abend
Thompson, Christopher	Bruker Daltonics, Billerica, MA, USA	Poster Session Montag Abend
Thompson, Christopher J.	Bruker Daltonics Inc., Billerica, MA, USA	Grundlagen und Instrumentelle Entwicklungen II
Tissier, Alain	Department of Cell and Metabolic Biology, Leibniz Institute of Plant Biochemistry (Halle/Saale)	Analytische Anwendungen II
Torres, Tomás	Universidad Autónoma de Madrid, Spain; Instituto Madrileño de Estudios Avanzados (IMDEA)-Nanociencia, Spain	Poster Session Montag Abend
Totzeck, Matthias	University Hospital Essen, Medical Faculty, West German Heart and Vascular Center,	Poster Session Montag Abend

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	Department of Cardiology and Department of Angiology, Germany	
Towers, Mark	Waters Corporation, United Kingdom	Bildgebende Massenspektrometrie
Traikov, Sofia	MPI of Cell Biology and Genetics, Dresden, Germany	Poster Session Montag Abend Vortragend
Treitz, Christian	AG Systematische Proteomforschung & Bioanalytik, Institut für Experimentelle Medizin, Christian-Albrechts-Universität zu Kiel, Kiel, Deutschland; Institut für Experimentelle Medizin, Uni Kiel	Poster Session Montag Abend Poster Session Montag Abend Vortragend
Treu, Axel	Universität Bayreuth, Deutschland	Poster Session Montag Abend Vortragend Poster Session Montag Abend
Trog, Sabrina	Humboldt-Universität zu Berlin, Deutschland	Poster Session Montag Abend Vortragend
Tudzynski, Paul	Institute of Plant Biology and Biotechnology, University of Münster, Germany	Poster Session Montag Abend
Turunen, Lotta	Department of Chemistry, NanoScience Center, University of Jyvaskyla, Finnland	Ionen Mobilität
Tyrasa, Swen	Analytik Jena AG, Jena, Germany	Poster Session Montag Abend
Uecker, Marina	Proteomics Group, Max-Planck-Institute of Experimental Medicine, 37075 Göttingen, Germany	Poster Session Montag Abend
Uetrecht, Charlotte	Heinrich-Pette-Institut, Hamburg, Deutschland; European XFEL GmbH, Schenefeld, Germany; Heinrich-Pette-Institute, Leibniz Institute for Experimental Virology, Hamburg, Germany	Poster Session Montag Abend Native Massespektrometrie Poster Session Montag Abend Poster Session Montag Abend
Uhl, Agnes	Friedrich-Alexander-University Erlangen-Nürnberg, Germany	Gasphasenreaktionen & Fragmentierungen II
Ulbrich, Anne	Universität Rostock, Deutschland	Poster Session Montag Abend Vortragend
Urlaub, Henning	Max Planck Institute for Biophysical Chemistry, Göttingen, Germany; University Medical Center Göttingen, Germany	Analytische Anwendungen II Poster Session Montag Abend
Uschold, Stephanie	Max Planck Institute for the Structure and Dynamics of Matter CFEL, Hamburg	Poster Session Montag Abend
Van Orden, Steve L.	Bruker Daltonics Inc., Billerica, MA, USA	Grundlagen und Instrumentelle Entwicklungen II
Van Soest, Remco	SCIEX, USA	Poster Session Montag Abend
VanOrden, Steve	Bruker Daltonics, Billerica, MA, USA	Poster Session Montag Abend
Vappiani, Johanna	Cellzome GmbH, Heidelberg	Proteine & Proteomics I
Vastenhouw, Nadine	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany, Deutschland	Proteine & Proteomics II
Vaudel, Marc	KG Jebsen Center for Diabetes Research, Department of Clinical Science, University of Bergen, Norway; Center for Medical Genetics and Molecular Medicine, Haukeland University Hospital, Bergen, Norway	MS-Informatik/Bioinformatik
Vendruscolo, Michele	University of Cambridge, United Kingdom	Native Massespektrometrie
Venne, A. Saskia	ISAS, Deutschland	Proteine & Proteomics II
Vennemann, Antje	IBE R&D gGmbH	Bildgebende Massenspektrometrie
Vens-Cappell, Simeon	University of Münster, Insitute for Hygiene, Münster, Germany; Interdisciplinary Center for Clinical Research (IZKF) Münster, Germany	Poster Session Montag Abend Poster Session Montag Abend Vortragend
Verhelst, Steven	ISAS, Deutschland; Department of Cellular and Molecular Medicine, Leuven, Belgium	Proteine & Proteomics II
Vetere, Alessandro	Max-Planck-Institut für Kohlenforschung, Deutschland	Grundlagen und Instrumentelle Entwicklungen II Vortragend
Vialaret, Jerome	Laboratoire de Biochimie et Protéomique Clinique, Institut de Médecine Régénératrice et de Biothérapie, CHU de Montpellier - Hôpital St. Eloi, Montpellier, France	Poster Session Montag Abend

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Vikhnina, Maria	Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry, Germany; Department of Biochemistry, St. Petersburg State University, Russia	Poster Session Montag Abend Vortragend
Villatoro, José	University of Potsdam, Germany; Bundesanstalt für Materialforschung und -prüfung, Germany; School of Analytical Sciences Adlershof, Germany	Poster Session Montag Abend Vortragend
Viner, Rosa	Thermo Fisher Scientific, San Jose, CA, USA	Poster Session Montag Abend
Vissers, Johannes PC	Waters Corporation, Wilmslow, United Kingdom	Poster Session Montag Abend Poster Session Montag Abend
Vitt, Stella	Max Planck Institute of Biophysics, Frankfurt	Poster Session Montag Abend
Vitz, Jürgen	Friedrich Schiller University Jena, Deutschland	Analytische Anwendungen I
Vogel, Sarah	Institute of Physiological Chemistry, Faculty of Medicine Carl Gustav Carus, Technical University Dresden, Germany	Poster Session Montag Abend
Vogt, Thomas	Department of Cell and Metabolic Biology, Leibniz Institute of Plant Biochemistry (Halle/Saale)	Analytische Anwendungen II
Volmer, Dietrich A.	Saarland University, Saarbrücken, Deutschland	Analytische Anwendungen I Klinische Diagnostik & Forensic Metabolomics Vortragend
von Bergen, Martin	Helmholtz-Centre for Environmental research (UFZ), Department of Molecular Systems Biology, Leipzig, Germany; University of Leipzig, Faculty of Biosciences, Pharmacy and Psychology, Leipzig, Germany; Department for Molecular Systems Biology, Helmholtz Centre for Environmental Research – UFZ, Leipzig, Germany	Poster Session Montag Abend Poster Session Montag Abend
von der Wellen, Jens	Bundeswehr Institute of Pharmacology and Toxicology	Poster Session Montag Abend Vortragend
von Helden, Gert	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland	Grundlagen und Instrumentelle Entwicklungen II Poster Session Montag Abend
Vosse, Christian	Westfälische Wilhelms-Universität Münster, Deutschland	Poster Session Montag Abend Vortragend
Vu Huu, Khanh	Johann Wolfgang Goethe-Universität, Deutschland	Poster Session Montag Abend Vortragend
Wachsmuth, Christian J.	University of Regensburg, Institute of Functional Genomics, Regensburg, Deutschland	Poster Session Montag Abend
Wagner, Anne	Cellzome GmbH, Heidelberg	Proteine & Proteomics I
Walter, Frederik	Bielefeld University, Bielefeld, Deutschland	Poster Session Montag Abend
Walter, Ulrich	Center for Thrombosis and Hemostasis, Universitätsklinikum der Johannes Gutenberg-Universität Mainz, Mainz, Germany;	Proteine & Proteomics I
Walters, David	Fort Collins Science Center, US Geological Survey, Fort Collins, USA	Bildgebende Massenspektrometrie
Wanczek, Karl Peter	Universität Bremen	Grundlagen und Instrumentelle Entwicklungen II
Wang, Nan	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster Session Montag Abend
Wang, Qing	Department of Plant Breeding, Justus Liebig University Giessen, Heinrich-Buff-Ring 26–32, 35392 Giessen, Germany	Metabolomics
Wang, Xiaohang	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster Session Montag Abend
Wang, Xuxiao	Max-Planck-Institut für Kohlenforschung, Deutschland	Gasphasenreaktionen & Fragmentierungen I Vortragend
Wang, Yuting	Center for Regenerative Therapies, Technical University Dresden, Dresden, Germany;	Lipide I Vortragend

Autor(en)	Organisation(en)	Session
	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany	
Warmbrunn, Vera	Friedrich-Alexander-University Erlangen-Nürnberg, Germany	Poster Session Montag Abend Vortragend
Warzok, Ulrike	Freie Universität Berlin	Ionen Mobilität Vortragend
Watz, Henrik	Pulmonary Research Institute at LungenClinic Großhansdorf, Wöhrendamm 80, 22927 Großhansdorf.; Airway Research Center North, German Center for Lung Research, Wöhrendamm 80, 22927 Großhansdorf, Germany	Lipide II
Weber, Marcus	Zuse Institute Berlin, Germany	Poster Session Montag Abend
Weibchen, Gunnar	Waters GmbH, Germany	Poster Session Montag Abend Vortragend Poster Session Montag Abend Vortragend
Weinmann, Wolfgang	Institute of Forensic Medicine, University of Bern; University of Bern, Institute of Forensic Medicine, Forensic Toxicology and Chemistry, Bühlstrasse 20, 3012 Bern, Switzerland; Universtität Bern, Institut für Rechtsmedizin, Forensische Toxikologie und Chemie, Switzerland	Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend
Weissflog, Jerrit	Max Planck Institute for Chemical Ecology, Jena, Germany	Poster Session Montag Abend Vortragend
Weller, Philipp	Hochschule Mannheim, Deutschland	Poster Session Montag Abend Poster Session Montag Abend
Wendt, Juergen	LECO European Application&Technology Center, Berlin, Germany	Poster Session Montag Abend Vortragend Grundlagen und Instrumentelle Entwicklungen II
Wendt, Karin	Bruker Daltonik GmbH, Deutschland	Poster Session Montag Abend
Werner, Hauke	Department of Neurogenetics, Max-Planck-Institute of Experimental Medicine, 37075 Göttingen, Germany	Poster Session Montag Abend
Weske, Sebastian	Georg-August-University Göttingen, Germany	Poster Session Montag Abend Vortragend
Wessjohann, Ludger A.	Leibniz-Institut für Pflanzenbiochemie, Abteilung Natur- und Wirkstoffchemie, Germany; Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry (Halle/Saale); Leibniz Institute of Plant Biochemistry, Department of Bioorganic Chemistry	Analytische Anwendungen II Analytische Anwendungen II Poster Session Montag Abend
Westphal, Dennis	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig, Germany	Poster Session Montag Abend Vortragend
Widdig, Anja	Universität Leipzig, Deutschland; Max-Planck-Institut für Evolutionäre Anthropologie, Leipzig, Deutschland; Deutsches Zentrum für integrative Biodiversitätsforschung, Leipzig, Deutschland; German Center for Integrative Biodiversity Research (iDiv), Germany	Poster Session Montag Abend Poster Session Montag Abend
Wiegelmann, Marcel	Institute for Hygiene, Biomedical Mass Spectrometry, University of Münster, Germany	Grundlagen und Instrumentelle Entwicklungen I Vortragend Poster Session Montag Abend
Wiemann, Martin	IBE R&D gGmbH	Bildgebende Massenspektrometrie
Wildgoose, Jason	Waters Corporation, Wilmslow, United Kingdom	Poster Session Montag Abend Poster Session Montag Abend
Wilharm, Thomas	ASG Analytik Service-Gesellschaft mbH, Neusäss	Grundlagen und Instrumentelle Entwicklungen II
Winter, Martin	Institute of Pathology, Christian-Albrechts-Universität, Kiel, Germany	Klinische Diagnostik & Forensic Vortragend
Witt, Matthias	Bruker Daltonik GmbH, Bremen, Germany	Grundlagen und Instrumentelle Entwicklungen II Poster Session Montag Abend
Wittig, Ilka	Goethe-Universität-Frankfurt	Proteine & Proteomics II

Autor(en)	Organisation(en)	Session
Wittig, Sabine	Interdisciplinary research center HALOmem, Martin Luther University Halle-Wittenberg, Kurt-Moses-Straße-3, 06120 Halle (Saale).	Poster Session Montag Abend Vortragend
Wohlfahrt, Sebastian	Helmholtz-Zentrum München,Deutschland	Poster Session Montag Abend
Wolf, Rainer	Competence Center Analytics, BASF SE, D-67056 Ludwigshafen	Poster Session Montag Abend Vortragend
Wolters-Eisfeld, Gerrit	University Medical Center Hamburg-Eppendorf, Deutschland	Poster Session Montag Abend Poster Session Montag Abend
Woolerton, Yvonne	Centre for Proteome Research, Institute of Integrative Biology, University of Liverpool, Liverpool, UK	Poster Session Montag Abend
Wozny, Katharina	Biochemie-Zentrum Heidelberg, Deutschland	Lipide I Vortragend Poster Session Montag Abend
Wrage, Jasmin	GALAB Laboratories GmbH, Deutschland	Poster Session Montag Abend Vortragend
Wu, Yiman	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster Session Montag Abend
Wulf, Helena	Universitätsklinikum Schleswig-Holstein, Deutschland	Klinische Diagnostik & Forensic
Wurlitzer, Marcus	University Medical Centre Hamburg-Eppendorf, Institute of Clinical Chemistry, Department for Mass Spectrometric Proteomics, Hamburg Germany	Poster Session Montag Abend
Wutkowski, Adam	Division of Bioanalytical Chemistry, Research Center Borstel, Parkallee 10, Borstel, Germany	Lipide I Vortragend
Xu, Xiaoma	Netherlands Forensic Institute, Forensic Chemistry – Chemical Identification Analysis, 2497 GB The Hague, Netherlands	Analytische Anwendungen I
Xu, Yun	Max-Planck-Institut für Kohlenforschung, Deutschland	Poster Session Montag Abend Vortragend
Yan, Hao	Heinrich Pette Institute, Leibniz Institute for Experimental Virology, Hamburg, Germany	Poster Session Montag Abend Vortragend Poster Session Montag Abend
Yates, Lisa M.	Princeton University	Proteine & Proteomics I
Yavor, Mikhail	Institute of Analytical instrumentation, Russian Academy of Sciences, Russia	Poster Session Montag Abend
Yefremova, Yelena	Proteome Center Rostock, Deutschland	Ionen Mobilität
Young, Phoebe	Goethe Universität Frankfurt, Deutschland	Poster Session Montag Abend Vortragend
Zahedi, René	Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund, Germany	Klinische Diagnostik & Forensic
Zahedi, René P.	ISAS, Deutschland	Proteine & Proteomics II Vortragend
Zahedi, Rene P.	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Deutschland	Proteine & Proteomics I
Zanni, Thomas	Markes International GmbH, Schleussnerstrasse 42, Frankfurt, Germany	Ionisationsmethoden
Zeissig, Sebastian	Center for Regenerative Therapies, Technical University Dresden, Dresden, Germany; Department of Medicine I, University Medical Center Dresden, Technical University Dresden, Dresden, Germany	Lipide I
Zeller, Martin	Thermo Fisher Scientific, Deutschland	Poster Session Montag Abend Poster Session Montag Abend
Zhao, Shuang	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster Session Montag Abend
Zheng, Xueyun	Pacific Northwest National Laboratory, USA	Ionen Mobilität
Zimmermann, Ralf	Helmholtz Zentrum Muenchen, Neuherberg; University of Rostock, Rostock	Grundlagen und Instrumentelle Entwicklungen II
Zimmermann, Ralf	Joint Mass Spectrometry Centre / Chair of Analytical Chemistry, University of Rostock, 18059 Rostock, Germany; HICE - Helmholtz Virtual of Complex Molecular Systems in Environmental Health – Aerosols and Health, www.hice-vi.eu; Cooperation Group Comprehensive Molecular Analytics, Helmholtz Zentrum München, 85764 Neuherberg, Germany;	Analytische Anwendungen I Ionisationsmethoden Poster Session Montag Abend Poster Session Montag Abend Poster Session Montag Abend

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	Universität Rostock, Deutschland; Helmholtz-Zentrum München, Deutschland; 2Joint Mass Spectrometry Centre Helmholtz-Zentrum München, Comprehensive Molecular Analytics (CMA), Neuherberg, Germany	
Zinn, Nico	Cellzome GmbH, Heidelberg	Proteine & Proteomics I Vortragend
Zuleger, Nikolaj	MPI of Cell Biology and Genetics, Dresden, Germany	Poster Session Montag Abend

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Autor(en)	Organisation(en)	Session
Abdelrahman, Hamada	Faculty of Agriculture, Cairo University	Poster
Ahrends, Robert	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Otto-Hahn-Str. 6b, 44227 Dortmund, Germany	DiN_1a, DiN_3a, MoV_1b, Poster
Ambach, Lars	Universtität Bern, Institut für Rechtsmedizin, Forensische Toxikologie und Chemie, Switzerland; Universität Ghent, Department of Bioanalysis, Laboratory of Toxicology, Belgium	Poster
Angelidou, Georgia	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig; Center for Biotechnology and Biomedicine, Universität Leipzig, Germany	MoV_1a
Angerer, Verena	Universitätsklinikum Freiburg, Institut für Rechtsmedizin, Forensische Toxikologie, Germany	Poster
Arlt, Christian	Institute of Pharmacy, Martin Luther University Halle-Wittenberg; Martin-Luther Universität Halle-Wittenberg, Deutschland	MiV_1a, MiV_3a Vortragend
Armeni, Marina	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig; Center for Biotechnology and Biomedicine, Universität Leipzig, Germany	MoV_1a
Arndt, Birgit	Institute of Food Chemistry, University of Münster, Germany	Poster
Arnhold, Jürgen	University of Leipzig, Medical Faculty, Institute of Medical Physics and Biophysics, Härtelstrasse 16- 18, 04107 Leipzig, Germany	DiN_3a
Arnold, Anne	Goethe Universität Frankfurt, Deutschland	Poster Vortragend
Arrey, Tabiwang	Thermo Fisher Scientific, Deutschland	Poster Vortragend, Poster Vortragend
Asperger, Arndt	Bruker Daltonik GmbH, Bremen, Germany	MiV_2a, Poster Vortragend, Poster Vortragend
Augsburg, Martina	Medical Systems Biology Medical Faculty, TU Dresden, Dresden, Germany	MiV_1a
Auth, Thomas	Georg-August-Universität Göttingen, Deutschland	MoV_3b, Poster Vortragend
Ayet San Andrés, Samuel	II physikalisches Insitut, Justus-Liebig-Universität Gießen, Deutschland; GSI Darmstadt, Deutschland	Poster
Bader, Theresa	Helmholtz Zentrum München, Deutschland	MiV_2a
Baesmann, Carsten	Bruker Daltonik GmbH, Deutschland	Poster
Bagwan, Navratan	Centro Nacional de investigaciones Cardiovasculares Carlos III (CNIC), Melchor Fernandez Almagro 3, 28029 Madrid, Spain	MoV_1b
Bahr, Ute	Goethe-Universität-Frankfurt	MiV_1a, Poster
Bailey, Aaron	Thermo Fisher Scientific, USA	Poster
Bajic, Steve	Waters Corporation, United Kingdom	MoN_3a Vortragend
Baker, Erin	Pacific Northwest National Laboratory, USA	DiV_4a
Balcke, Gerd U.	Leibniz-Institut für Pflanzenbiochemie, Stoffwechsel- und Zellbiologie, Germany	DiV_3a
Baldwin, Ian T.	Max Planck Institute for Chemical Ecology, Department for Molecular Ecology, Jena, Germany	Poster
Bantscheff, Marcus	Cellzome GmbH, Heidelberg	MoN_1a
Barayeu, Uladzimir	University of Leipzig, Medical Faculty, Institute of Medical Physics and Biophysics, Härtelstrasse 16- 18, 04107 Leipzig, Germany	DiN_3a Vortragend
Bärenfänger, Melissa	Uni Hamburg, Deutschland	Poster Vortragend

Autor(en)	Organisation(en)	Session
Barsch, Aiko	Bruker Daltonik GmbH, Deutschland	Poster, Poster, Poster, Poster
Bartelmus, Christian	Hoffmann la Roche AG, Schweiz	Poster Vortragend
Bartels, Benjamin	Research Group Mass spectrometry/Proteomics, Max Planck Institute for Chemical Ecology	MoV_3b Vortragend
Barth, Christof	Justus-Liebig-Universität Gießen, Deutschland	Poster, Poster Vortragend
Baschung, Yannick	Steinbeis Centre Biopolymer Analysis & Biomedical Mass Spectrometry, Rüsselsheim, Germany; Proteome Center, Institute of Immunology, University of Rostock, Rostock, Germany	Poster Vortragend
Bauer, Anna	GALAB Laboratories GmbH, Deutschland	DiN_1a
Baumgarten, Sigrid	Shimadzu Europa GmbH, Deutschland	Poster
Bayer, Malte	WWU Münster	MiV_1a Vortragend
Baykut, Gökhan	Bruker Daltonik GmbH, Bremen, Germany	MiV_2a, Poster
Becana, Manuel	Estación Experimental de Aula Dei, Consejo Superior de Investigaciones Científicas (CSIC), Department of Plant Nutrition	Poster
Becher, Simon	Institut für Anorganische und Analytische Chemie; Justus-Liebig-Universität Gießen	Poster
Beck, Florian	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Deutschland	MoN_1a
Beck, Sebastian	Humboldt-Universität zu Berlin	Poster, Poster
Becker, Alexander	Christian-Albrechts-Universität zu Kiel, Deutschland	Poster Vortragend
Becker, René	Humboldt-Universität zu Berlin, Institut für Chemie, Deutschland	Poster Vortragend
Begemann, Nora	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	Poster Vortragend
Beitz, Toralf	University of Potsdam, Germany	Poster
Benninghaus, Thomas	University Medical Center Hamburg-Eppendorf, Deutschland	Poster
Berg, Christian	Bruker Daltonics Inc., Billerica, MA, USA	MiV_2a, Poster
Bergamini, Giovanna	Cellzome GmbH, Heidelberg	MoN_1a
Bergmann, Julian	II physikalisches Insitut, Justus-Liebig-Universität Gießen, Deutschland	Poster Vortragend
Beynon, Robert	Centre for Proteome Research, Institute of Integrative Biology, University of Liverpool, Liverpool, UK	Poster
Bhandari, Dhaka Ram	Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, Heinrich-Buff-Ring 17, 35392 Giessen, Germany; Justus Liebig University Giessen, Institute of Inorganic and Analytical Chemistry	DiV_2a Vortragend, MoV_2a
Bierstedt, Andreas	Bundesanstalt für Materialforschung und -prüfung, Deutschland	Poster Vortragend
Bilova, Tatiana	Leibniz-Institut für Pflanzenbiochemie, Abteilung Natur- und Wirkstoffchemie, Germany; Universität Leipzig, Fakultät für Chemie und Mineralogie, Germany; Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry (Halle/Saale); Faculty of Chemistry and Mineralogy, Universität Leipzig; Department of Plant Physiology and Biochemistry, St. Petersburg State University, Russia; Leibniz Institute of Plant Biochemistry, Department of Bioorganic Chemistry	DiV_3a, DiV_3a Vortragend, Poster, Poster
Birkemeyer, Claudia	Universität Leipzig, Fakultät für Chemie und Mineralogie, Germany; Faculty of Chemistry and Mineralogy,	DiV_3a, DiV_3a, MoN_3a, Poster, Poster Vortragend, Poster

Autor(en)	Organisation(en)	Session
	Universität Leipzig; Universität Leipzig, Deutschland	
Bittner, Marian	Freie Universität Berlin, Institute of Pharmacy, Pharmaceutical Biology	Poster Vortragend
Blaum, Bärbel	Interfaculty Institute of Biochemistry, University of Tübingen, Tübingen, Germany	Poster
Böcker, Sebastian	Chair for Bioinformatics, Friedrich Schiller University Jena	MoV_3b
Bomgarden, Ryan	Thermo Fisher Scientific, Rockford, IL, USA	Poster
Bookmeyer, Christoph H. M.	Institute for Hygiene, University of Münster, Robert-Koch-Str. 41, 48149 Münster, Germany	Poster Vortragend
Boosfeld, Jochen	Bruker Daltonik GmbH, Deutschland	Poster Vortragend, Poster Vortragend
Borchard, Nils	Center for International Forestry Research, Indonesia	Poster
Borovinskaya, Olga	TOFWERK, Switzerland	Poster
Borowski, Kathrin	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	Poster
Boskamp, Marcel	Institute for Hygiene, University of Münster, Germany	Poster, Poster Vortragend
Bowers, Michael T.	University of California, Santa Barbara, USA	Poster
Brandt, Wolfgang	Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry (Halle/Saale)	DiV_3a
Brauch, Dominic	Faculty of Chemistry and Mineralogy, Universität Leipzig; Leibniz Institute of Plant Genetics and Crop Plant Research (Stadt Seeland)	DiV_3a
Brockmann, Eike Ulrich	Institute for Hygiene, Biomedical Mass Spectrometry, University of Münster, Germany	Poster Vortragend
Brogly, Sophie	Hoffmann la Roche AG, Schweiz	Poster
Brosch, Mario	Department of Medicine I, University Medical Center Dresden, Technical University Dresden, Dresden, Germany	MoV_1b
Brüchert, Stefan	Johann Wolfgang Goethe-Universität, Deutschland	Poster
Brügger, Britta	Biochemie-Zentrum Heidelberg, Deutschland	MoV_1a, Poster
Bruns, Heiko	University Hospital Erlangen, Deutschland	DiV_2a
Bücher, Katharina	Institute for Organic and Macromolecular Chemistry Heinrich-Heine-University Düsseldorf, Düsseldorf Germany	Poster
Buchholz, Frank	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany, Deutschland; Medical Systems Biology Medical Faculty, TU Dresden, Dresden, Germany	MiV_1a
Bukowski, Nick	Markes International, Gwaun Elai Medi-Science Campus, Llantrisant, RCT, Wales, United Kingdom	MoN_3a
Bunse, Christian	Shimadzu Deutschland GmbH, Deutschland	Poster Vortragend
Burkhart, Julia M.	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Deutschland	MoN_1a
Burmester, Ulrike	Bruker Daltonik GmbH, Deutschland	Poster Vortragend, Poster Vortragend
Busse, Frederik	Max Planck Institut für Struktur und Dynamik der Materie, Hamburg, Deutschland	Poster Vortragend
Bussmann, Tanja	Research and Development, Beiersdorf AG, Hamburg	Poster
Butter, Falk	Institute of Molecular Biology, Deutschland	MoN_2a Vortragend
Buzatto, Adriana	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster
Calleri, Enrica	Department of Drug Sciences, University of Pavia, Pavia, Italy	Poster

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Campidelli, Stéphane	LICSEN, NIMBE, CEA, CNRS, Université Paris-Saclay, France	DiV_1a
Cannistraci, Carlo V.	Biomedical Cybernetics Group, Biotechnology Center, Technical University Dresden, Dresden, Germany	MoV_1b
Cassidy, Liam Arron	AG Systematische Proteomforschung & Bioanalytik, Institut für Experimentelle Medizin, Christian-Albrechts-Universität, Kiel	Poster, Poster Vortragend
Castro-Perez, Jose	Waters Corporation, Milford, MA	Poster
Causon, Tim	BOKU Wien, Österreich	DiV_4a Vortragend
Chait, Brian T.	The Rockefeller University, New York, USA	WP Vortragend
Chantseva, Veronika	Department of Plant Physiology and Biochemistry, St. Petersburg State University	Poster Vortragend
Chen, Yu-Ju	Academia Sinica, School of Chemistry, Taipei, Taiwan	Poster, Poster
Chernev, Aleksandar	Max Planck Institute for Biophysical Chemistry, Göttingen, Germany	DiV_3a, Poster
Chervet, Jean-Pierre	ANTEC, Leyden	Poster
Ciucci, Sara	Biomedical Cybernetics Group, Biotechnology Center, Technical University Dresden, Dresden, Germany; Lipotype GmbH, Dresden, Germany	MoV_1b
Claassen, Christin	GALAB Laboratories GmbH, Deutschland	Poster
Claude, Emmanuelle	Waters Corporation, United Kingdom	MoV_2b
Clemen, Martin	Christian-Albrechts-Universität zu Kiel, Institut für Physikalische Chemie, Max-Eyth-Str. 1, 24118 Kiel, Deutschland	MoV_3a Vortragend
Coliva, Giulia	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig; Center for Biotechnology and Biomedicine, Universität Leipzig, Germany	MoV_1a, Poster Vortragend
Colombo, Simone	Mass Spectrometry Centre, Department of Chemistry & QOPNA, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal	Poster
Coman, Cristina	Leibniz-Institut für Analytische Wissenschaften – ISAS e.V., Germany	Poster Vortragend
Conway, Debra	Analytik Jena AG, Jena, Germany	Poster
Cornett, Shannon	Bruker Daltonics, Billerica, MA, USA	Poster
Cramer, Benedikt	Institute of Food Chemistry, University of Münster, Germany	Poster
Crawford, Elizabeth	Saarland University, Saarbrücken, Deutschland	MoN_2a Vortragend
Crecelius, Anna C.	Friedrich Schiller University Jena, Deutschland	MoN_2a Vortragend
Creutznacher, Robert	Institute of Chemistry, University of Lübeck, Lübeck, Germany	Poster
Crone, Barbara	Institut für Anorganische und Analytische Chemie, Universität Münster, Deutschland	MoV_2b Vortragend
Czech, Hendryk	Universität Rostock, Deutschland	MoN_3a Vortragend
Damoc, Eugen	Thermo Fisher Scientific, Deutschland	Poster, Poster
Danne-Rasche, Niklas	Leibniz Institut für Analytische Wissenschaften ISAS e.V.	MoV_1b Vortragend
Danquah, Bright D.	Proteome Center Rostock, Deutschland	DiV_4a
Danz, Norbert	Fraunhofer Institute for Applied Optics and Precision Engineering IOF	MoV_3b
Darland, Ed	Agilent Technologies, Santa Clara, USA	DiV_4a
De Angelis, Francesco	Dipart. di Sci. Fisiche e Chimiche, Università degli Studi dell'Aquila, Via Vetoio, Coppito, 67100 L'Aquila, Italy	MoV_3a
de Bruyn, René	Netherlands Forensic Institute, Forensic Chemistry – Chemical Identification Analysis, 2497 GB The Hague, Netherlands	MoN_2a

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Decker, Petra	Bruker Daltonik GmbH, Deutschland	Poster
Dedishov, Ruslan	Markes International GmbH, Schleussnerstrasse 42, Frankfurt, Germany	MoN_3a
Dell'Aica, Margherita	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Deutschland	MoN_1a
Denno, Yvonne	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	Poster
Desbenoit, Nicholas	Universität Bayreuth, Deutschland	Poster
Desbenoit, Nicolas	Chair of Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth, Germany	Poster, MoV_2b
Dettmer, Katja	University of Regensburg, Institute of Functional Genomics, Regensburg, Deutschland	Poster
Diarra, David	Oil-Wärme-Institut GmbH, Herzogenrath, Deutschland	Poster
Dickel, Timo	II physikalisches Insitut, Justus-Liebig-Universität Gießen, Deutschland; GSI Darmstadt, Deutschland	Poster
DiConza, Giusy	Laboratory of Molecular Oncology and Angiogenesis, Vesalius Research Center, Leuven, Belgium	MoV_4b
Didio, Anna	Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry; Department of Biochemistry, St. Petersburg State University	Poster
Dietrich, Dörthe	Westfälische Wilhelms-Universität Münster	MoV_2a Vortragend
Ding, Xuelu	Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen	MoN_3a Vortragend
Dinse, Martin	PerkinElmer LAS (Germany) GmbH, Deutschland	Poster Vortragend
Dirk, Tänzler	Martin-Luther-University Halle-Wittenberg, Institute of Pharmacy, Department of Pharmaceutical Chemistry and Bioanalytics, Germany	Poster
Disko, Ulrich	Forschungszentrum Jülich, Deutschland	Poster
Dojahn, Joerg	SCIEX, Deutschland	Poster Vortragend
Domingues, M. Rosario	Mass Spectrometry Centre, Department of Chemistry & QOPNA, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal	Poster
Domingues, Pedro	Mass Spectrometry Centre, Department of Chemistry & QOPNA, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal	Poster
Dopstadt, Julian	Institute of Food Chemistry, University of Münster, Germany	Poster
Dral, Pavlo O.	Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany	DiV_1a
Drechsel, David	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany, Deutschland; Present address: IMP Research Institute of Molecular Pathology, 1030 Vienna, Austria	MiV_1a
Dreger, Mathias	caprotec bioanalytics GmbH	MoN_1a
Dreisewerd, Klaus	Institute for Hygiene, University of Münster, Germany; Interdisciplinary Center for Clinical Research (IZKF), University of Münster, Germany; University of Münster, Institute of Hygiene, Biomedical Mass Spectrometry, Germany; Institute for Hygiene, University of Münster, Robert-Koch-Str. 41, 48149 Münster, Germany	Poster, Poster, Poster, Poster, Poster, Poster, MoV_3b, Poster, Poster
Drewello, Thomas	Friedrich-Alexander-University Erlangen-Nürnberg, Germany	DiV_1a, DiV_1a, Poster, Poster, Poster

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Dreyer, Benjamin	University Medical Center Hamburg Eppendorf, Deutschland	Poster Vortragend, Poster
Dülcks, Thomas	Universität Bremen, Deutschland	Poster Vortragend
Dunn, Adrian	Departments of Platform Technology & Science, GlaxoSmithKline, Stevenage, UK	Poster
Dürr, Maximilian	Friedrich-Alexander-University Erlangen-Nürnberg, Deutschland	Poster
Duschl, Wolfgang J.	Christian-Albrechts-Universität zu Kiel, Deutschland	Plenarvortrag 4 Vortragend
Dwayne Miller, R. J.	Max Planck Institute for the Structure and Dynamics of Matter CFEL, Hamburg	Poster
Easterling, Michael L.	Bruker Daltonics, Billerica, MA, USA	Poster, MiV_2a
Eble, Johannes	Institut für Physiologische Chemie und Pathobiochemistry, Universität Münster, Deutschland	Poster
Eckelmann, Paula	Federal Criminal Police Office, Forensic Institute, 65193 Wiesbaden, Germany; Justus-Liebig-University Giessen, Institute of Food Chemistry and Food Biotechnology, 35392 Giessen, Germany	MoN_2a
Eckey, Kevin	Universität Münster, Deutschland	Poster Vortragend
Edler, Stefan	LAS Perkinelmer GmbH, Deutschland	Poster Vortragend
Eggers, Lars Florian	Research Center Borstel, Division of Bioanalytical Chemistry, Parkallee 1-40, D-23845 Borstel, Germany.	DiN_3a Vortragend
Eggert, Dennis	Heinrich Pette Institute, Leibniz Institute for Experimental Virology, Hamburg	Poster
Eiersbrock, Fabian	Institute for Hygiene, University of Münster, Germany	Poster Vortragend, Poster
Einspanier, Almuth	Universität Leipzig, Deutschland	Poster
El-Khatib, Ahmed	Humboldt-Universität zu Berlin, Institut für Chemie, Deutschland	Poster, Poster
Enders, Claudia	Merck KGaA, Frankfurter Str. 250, 64293 Darmstadt, Germany	Poster
Engeser, Marianne	Universität Bonn, Deutschland	DiV_1a Vortragend, Poster
Ermler, Ulrich	Max Planck Institute of Biophysics, Frankfurt	Poster
Esch, Patrick	Institute of Inorganic and Analytical Chemistry, Justus-Liebig-University, Giessen, Germany	MoV_1b Vortragend
Escher, Beate	Helmholtz-Centre for Environmental research (UFZ), Department of Cell Toxicology, Leipzig, Germany	Poster
Esfeld, Sonja	University Hospital Essen, Medical Faculty, West German Heart and Vascular Center, Department of Cardiology and Department of Angiology, Germany	Poster
Etienne, Chris	Thermo Fisher Scientific, Rockford, IL, USA	Poster
Faelth-Savitski, Maria	Cellzome GmbH, Heidelberg	MoN_1a
Fagbadebo, Funmilayo	Leibniz-Institut für Pflanzenbiochemie, Abteilung Natur- und Wirkstoffchemie, Germany	DiV_3a
Farmani, Zahra	Bio-film Center Universität Duisburg-Essen; Max-Planck-Institut für Kohlenforschung, Germany	Poster Vortragend
Fatangare, Amol	Chair of Bioanalytical Sciences and Food Analysis, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth, Germany	MoV_2b, Poster Vortragend
Fazel, Ramin	The University of Tehran, Iran; Universitätsklinikum Hamburg-Eppendorf, Germany	DiV_3a Vortragend
Fedorova, Maria	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig, Germany; Center for Biotechnology and Biomedicine, Universität Leipzig, Germany	Poster, MoV_1a Vortragend, Poster

Autor(en)	Organisation(en)	Session
Fiedler, Dorothea	Leibniz-Institut für molekulare Pharmakologie (FMP), Deutschland; Humboldt-Universität zu Berlin; Princeton University	MoN_1a
Fielitz, Davor	Shimadzu Deutschland GmbH, Deutschland	Poster Vortragend
Firl, Nina	Shimadzu Deutschland GmbH, Deutschland	Poster
Fischer, Michael	Helmholtz-Zentrum München,Deutschland	Poster
Fischer, Moritz	Universität zu Köln, Deutschland	Poster Vortragend
Fischle, Wolfgang	Max Planck Institute for Biophysical Chemistry, Göttingen, Germany; KAUST, Saudi Arabia	DiV_3a
Fjeldsted, John	Agilent Technologies, Santa Clara, USA	DiV_4a
Flemmig, Jörg	University of Leipzig, Medical Faculty, Institute of Medical Physics and Biophysics, Härtelstrasse 16- 18, 04107 Leipzig, Germany	DiN_3a
Folberth, Julica	University of Lübeck, Germany	DiV_2a Vortragend
Franken, Holger	Cellzome GmbH, Heidelberg	MoN_1a
Franz, Florian	Universitätsklinikum Freiburg, Institut für Rechtsmedizin, Forensische Toxikologie, Germany	Poster
Franzke, Joachim	Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V.	MoN_3a
Fraune, Sebastian	Zoologisches Institut, Uni Kiel	Poster
Frensemeier, Lisa	Universität Münster, Deutschland	MoV_4a Vortragend
Freund, Christian	Institut für Chemie und Biochemie, Freie Universität Berlin, Deutschland	Poster
Friedrich, Jochen	Bruker Daltonik GmbH, Bremen, Germany	MiV_2a Vortragend, Poster
Frolov, Andrej	Leibniz-Institut für Pflanzenbiochemie, Abteilung Natur- und Wirkstoffchemie, Germany; Universität Leipzig, Fakultät für Chemie und Mineralogie, Germany	DiV_3a Vortragend
Frolov, Andrej	Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry (Halle/Saale); Faculty of Chemistry and Mineralogy, Universität Leipzig; Leibniz Institute of Plant Biochemistry, Department of Bioorganic Chemistry	DiV_3a, Poster, Poster, Poster
Fuchs, M.	2Joint Mass Spectrometry Centre Helmholtz-Zentrum München, Comprehensive Molecular Analytics (CMA), Neuherberg, Germany	Poster
Fuchs, Sabine	Klinik für Unfallchirurgie und Traumatologie, Experimentelle Unfallchirurgie, UKSH, Kiel	Poster
Fuchser, Jens	Bruker Daltonik GmbH, Bremen, Germany	MiV_2a, Poster
Fuetterer, Arne	Bruker Daltonik GmbH, Germany	Poster
Fufezan, Christian	Institute for Biology and Biotechnology of Plants, University Münster, Münster, Germany;	MoN_1a
Fuh, Marceline Manka	University Medical Centre Hamburg-Eppendorf, Institute of Clinical Chemistry, Department for Mass Spectrometric Proteomics, Hamburg Germany	Poster Vortragend
Furrer, Julien	Department of Chemistry and Biochemistry, University of Bern	Poster
Gabelica, Valérie	Inserm, CNRS, Université de Bordeaux, Laboratoire "Acides Nucléiques, Régulations Naturellee et Artificielle" (ARNA, U1212, UMR5320), IECB, Pessac, France	Plenarvortrag 2 Vortragend
Gabelle, Audrey	Laboratoire de Biochimie et Protéomique Clinique, Institut de Médecine Régénératrice et de Biothérapie, CHU de Montpellier - Hôpital St. Eloi, Montpellier, France; Centre Mémoire Ressources Recherche, CHU Montpellier, hôpital Gui de Chauliac, Montpellier, France	Poster

Autor(en)	Organisation(en)	Session
Gade, Stephan	Cellzome GmbH, Heidelberg	MoN_1a
Gallaspy, Alan	PerkinElmer LAS (Germany) GmbH, Deutschland	Poster
Galyamova, Aigerim	Pennsylvania State University, USA	MoN_3a
Gambaryan, Stepan	Sechenov Institute of Evolutionary Physiology and Biochemistry, Russian Academy of Sciences, Saint Petersburg, Russia;	MoN_1a
Gaquerel, Emmanuel	Centre for Organismal Studies Heidelberg, University of Heidelberg, Germany	Poster
Garbeva, Paolina	Department of Microbial Ecology, Netherlands Institute of Ecology, Wageningen, The Netherlands	DiN_2a
Garcia Alai, Maria Marta	European Molecular Biology Laboratory (EMBL), Hamburg, Germany	MiV_3a
Geiger, Jörg	Interdisciplinary Bank of Biomaterials and Data, Würzburg, Germany;	MoN_1a
Geissel, Hans	II physikalisches Insitut, Justus-Liebig-Universität Gießen, Deutschland; GSI Darmstadt, Deutschland	Poster
Gentzel, Marc	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany, Deutschland; Present address: Center for Molecular and Cellular Bioengineering, TU Dresden, 01307 Germany	MiV_1a
Gerbig, Stefanie	Justus Liebig University, Gießen, Deutschland	MoN_2a, Poster Vortragend
Gerbig, Stefanie	Justus-Liebig-Universität Gießen, Institut für Anorganische und Analytische Chemie	MoN_2a
Gerhardt, Natalie	Hochschule Mannheim, Deutschland	Poster Vortragend
Gethings, Lee	Waters Corporation, Wilmslow, United Kingdom	Poster, Poster
Gethings, Lee A	Waters, Wilmslow, UK	Poster, Poster
Gewinner, Sandy	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland	MiV_2a
Gieras, Anna	European Molecular Biology Laboratory (EMBL), Hamburg, Germany	MiV_3a
Glocker, Michael	Proteome Center, Institute of Immunology, University of Rostock, Rostock, Germany	Poster
Glocker, Michael O.	Proteome Center Rostock, Deutschland	DiV_4a Vortragend
Göbel, Michael	Goethe-Universität Frankfurt, Deutschland	MiV_3a
Goldmann, Torsten	Pathology of the University Hospital of Lübeck and the Research Center Borstel, Clinical and Experimental Pathology, 23538 Lübeck and 23845 Borstel, Germany.; Airway Research Center North, German Center for Lung Research, Wöhrendamm 80, 22927 Großhansdorf, Germany	DiN_3a
Golghalyani, Vahid	Goethe-Universität-Frankfurt	MiV_1a Vortragend, Poster
Gonzalez Florez, Ana Isabel	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland	MiV_2a
Goseli, Christoph	Bruker BioSpin, Fällanden, Switzerland	Poster
Gosteli, Christoph	Bruker BioSpin AG, Fällanden, Switzerland	MiV_2a
Göth, Melanie	Freie Universität Berlin, Deutschland; Fritz-Haber-Institut Berlin, Deutschland	MiV_3a Vortragend
Gottfried, Sebastian	Waters Corporation, United Kingdom	MoV_2b Vortragend
Gottwald, Sven	Department of Plant Breeding, Justus Liebig University Giessen, Heinrich-Buff-Ring 26–32, 35392 Giessen, Germany	DiV_2a
Götze, Michael	Institute of Biochemistry, Martin Luther University Halle-Wittenberg	MiV_1a
Grafinger, Katharina	Universtität Bern, Institut für Rechtsmedizin, Forensische Toxikologie und Chemie, Switzerland	Poster Vortragend

Autor(en)	Organisation(en)	Session
Grevelding, Christoph	Justus-Liebig-Universität Gießen, Institut für Parasitologie	MoN_2a
Grishina, Tatiana	Universität St. Petersburg, Lehrstuhl Biochemie, Russia; Department of Biochemistry, St. Petersburg State University	DiV_3a, Poster
Groessl, Michael	Tofwerk, Uttigenstrasse 22, CH-3600 Thun, Switzerland	DiV_4a, Poster
Gröger, Thomas	Helmholtz Zentrum Muenchen, Neuherberg	MiV_2a
Grosche, Julius	Institut für Physiologische Chemie und Pathobiochemistry, Universität Münster, Deutschland	Poster
Gross, Jürgen	Universität Heidelberg, Deutschland	Poster Vortragend
Grotemeyer, Jürgen	Christian-Albrechts-Universität zu Kiel, Deutschland; Christian-Albrechts-Universität zu Kiel, Institut für Physikalische Chemie, Max-Eyth-Str. 1, 24118 Kiel, Deutschland	DiV_1a, MoV_3a, Poster, Poster, Poster, Poster
Gruber, Uschi	caprotec bioanalytics GmbH	MoN_1a
Grübner, Isabell	Goethe Universität Frankfurt, Deutschland	Poster
Grutters, Michiel	Netherlands Forensic Institute, Forensic Chemistry – Chemical Identification Analysis, 2497 GB The Hague, Netherlands	MoN_2a
Grützmacher, Hans-Friedrich	Department of Chemistry, Bielefeld University	Poster, Poster
Güttler, Bernd	Physikalisch-Technische-Bundesanstalt, Deutschland	Poster
Habchi, Johnny	University of Cambridge, United Kingdom	MiV_3a
Hachenberger, Yves U.	Humboldt-Universität zu Berlin	Poster Vortragend
Hachmöller, Oliver	Institute of Inorganic and Analytical Chemistry, University of Münster, Münster, Germany	MoV_4a Vortragend
Hädener, Marianne	University of Bern, Institute of Forensic Medicine, Forensic Toxicology and Chemistry, Bühlstrasse 20, 3012 Bern, Switzerland	Poster Vortragend
Hage, Christoph	Martin-Luther-Universität Halle-Wittenberg, Deutschland	DiV_1a Vortragend, Poster
Hagenhoff, Sebastian	Westfälische Wilhelms-Universität Münster	MoN_3a Vortragend
Hahm, Heung Sik	Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Potsdam, Deutschland	MiV_2a
Hahn, Bill	PerkinElmer LAS (Germany) GmbH, Deutschland	Poster
Hahn, Stefanie	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	Poster
Hahn, Uwe	Universidad Autónoma de Madrid, Spain; University of Strasbourg and CNRS, European School for Chemistry, Polymers and Materials (ECPM), France	Poster
Hakelberg, Matthias	caprotec bioanalytics GmbH	MoN_1a
Hamester, Meike	Bruker Daltonik GmbH, Germany	Poster
Han, Wei	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster
Hann, Stephan	BOKU Wien, Österreich	DiV_4a
Hannich, Thomas	University of Geneva, Department of Biochemistry	MoV_2a
Hansen, Nils-Owe	Max Planck Institute for the Structure and Dynamics of Matter	Poster, Poster, Poster, Poster
Hansman, Grant	DKFZ and Department of Infectious Diseases and Virology University of Heidelberg, Heidelberg, Germany	Poster
Hardy, Neil	Departments of Platform Technology & Science, GlaxoSmithKline, Stevenage, UK	Poster
Hart, Philippa J.	Waters Corporation, United Kingdom	MoV_2b

Autor(en)	Organisation(en)	Session
Hartmann, Laura	Institute for Organic and Macromolecular Chemistry Heinrich-Heine-University Düsseldorf, Düsseldorf Germany	Poster
Haslam, Carl	Departments of Platform Technology & Science, GlaxoSmithKline, Stevenage, UK	Poster
Hayen, Heiko	Westfälische Wilhelms-Universität Münster	MoN_3a, Poster
Hayen, Heiko	WWU Münster, Deutschland; Westfälische Wilhelms-Universität Münster, Deutschland	DiV_2a, Poster
Heber, Volker	PerkinElmer, Deutschland	Poster Vortragend
Heck, Albert	Universiteit Utrecht, The Netherlands	Poster
Heemskerk, Johan W. M.	Department of Biochemistry, Cardiovascular Research Institute Maastricht, Maastricht University, The Netherlands;	MoN_1a
Heeren, Ron M.A.	Maastricht University, Niederlande	Plenarvortrag 1 Vortragend
Heidemann, Johannes	Heinrich-Pette-Institute, Leibniz Institute for Experimental Virology, Hamburg, Germany; Heinrich-Pette-Institut, Hamburg, Deutschland	MiV_3a Vortragend, Poster
Heikaus, Laura	University Medical Center Hamburg-Eppendorf, Deutschland	Poster
Heikaus de Figueiredo, Laura	University Medical Center Hamburg Eppendorf, Deutschland	MiV_1a Vortragend
Heiles, Sven	Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen	MoN_3a, MoV_1b, Poster Vortragend
Heiling, Sven	Max Planck Institute for Chemical Ecology, Department for Molecular Ecology, Jena, Germany	Poster
Heimerl, Jule	Humboldt-Universität zu Berlin, Institut für Chemie, Deutschland	Poster
Heintze, Christoph	B-CUBE Center for Molecular Bioengineering, Dresden, Deutschland	MiV_3a
Helle, Niklas	Universität Kiel, Deutschland	Poster Vortragend
Hellwig, Nils	Goethe-University Frankfurt/Main, Deutschland; Institut für Physikalische und Theoretische Chemie, Goethe-Universität Frankfurt	Poster, Poster Vortragend
Hempel, Ute	Institute of Physiological Chemistry, Faculty of Medicine Carl Gustav Carus, Technical University Dresden, Germany	Poster
Hendgen-Cotta, Ulrike B.	University Hospital Essen, Medical Faculty, West German Heart and Vascular Center, Department of Cardiology and Department of Angiology, Germany	Poster
Hendrikse, Jeanet	Netherlands Forensic Institute, Forensic Chemistry – Chemical Identification Analysis, 2497 GB The Hague, Netherlands	MoN_2a
Henkel, Corinna	Bruker Daltonik GmbH, Bremen, Germany	MiV_2a
Henrion, André	Physikalisch-Technische-Bundesanstalt, Deutschland	Poster
Hense, Genia	Goethe Universität Frankfurt, Deutschland	Poster
Herfurth, Uta M.	Universität Leipzig, Fakultät für Chemie und Mineralogie, Germany	DiV_3a
Hinz, Klaus Peter	Justus-Liebig Universität Giessen, Deutschland	Poster, Poster Vortragend
Hirtz, Christophe	Laboratoire de Biochimie et Protéomique Clinique, Institut de Médecine Régénératrice et de Biothérapie, CHU de Montpellier - Hôpital St. Eloi, Montpellier, France	Poster
Hitzenberger, Jakob F.	Friedrich-Alexander-University Erlangen-Nürnberg, Germany	DiV_1a Vortragend, DiV_1a
Hoehenwarter, Wolfgang	Proteome Analytics Research Group, Leibniz Institute of Plant Biochemistry	Poster
Hoffmann, Christian	Free Floater (Junior) Research Group Applied Synthetic Biology, Georg-August University Göttingen, Institute for	Poster

Autor(en)	Organisation(en)	Session
	Microbiology and Genetics, 37077 Göttingen, Germany	
Hoffmann, Jan	University of Frankfurt, Deutschland	MiV_3a, Poster
Hoffmann, Ralf	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig, Germany; Center for Biotechnology and Biomedicine, Universität Leipzig, Germany	Poster, MoV_4a
Hoffmann, Waldemar	Freie Universität Berlin; Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin	DiV_4a, Poster Vortragend, MiV_2a
Hofmann, Diana	Forschungszentrum Jülich, Deutschland	Poster Vortragend
Hofmann, Tommy	Interdisciplinary research center HALOmem, Martin Luther University Halle-Wittenberg, Kurt-Moses-Straße-3, 06120 Halle (Saale).; Helmholtz-Centre for Environmental research (UFZ), Department of Molecular Systems Biology, Leipzig, Germany; HALOmem, Halle (Saale), Germany	MoV_1a Vortragend, Poster
Holterhus, Paul-Martin	Universitätsklinikum Schleswig-Holstein, Deutschland	MoV_4b
Hooton, Kevin	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster
Horner, Gerhard	Five Technologies GmbH, Frauenstrasse 22, 80469 Munich, Germany	MoN_3a Vortragend
Hoyes, John	Waters Corporation, Wilmslow, United Kingdom	Poster
Hübner, Florian	Institute of Food Chemistry, University of Münster, Germany	Poster
Hughes, Chris	Waters Corporation, Wilmslow, United Kingdom	Poster, Poster
Humpf, Hans-Ulrich	Institute of Food Chemistry, University of Münster, Germany	Poster, Poster
Hunger, Doreen	2Department of Microbiology, Institute of Biology, Martin-Luther University Halle-Wittenberg, Halle (Saale), Germany	Poster
Hunter, Christie	SCIEX, USA	Poster
Hutterli, Manuel	TOFWERK, Schweiz	Poster
Iacobucci, Claudio	UMR CNRS 6521, Université de Bretagne Occidentale, 6 Av.Le Gorgeu, 29200 Brest, France; Institute of Pharmacy, Martin-Luther University Halle-Wittenberg, Halle/Saale, Germany, Deutschland	MoV_3a Vortragend
Ickert, Stefanie	Bundesanstalt für Materialforschung- und prüfung, Deutschland	Poster Vortragend
Ihling, Christian	Institute of Pharmacy, Martin Luther University Halle-Wittenberg; Martin-Luther Universität Halle-Wittenberg, Deutschland; Martin-Luther-University Halle-Wittenberg, Institute of Pharmacy, Department of Pharmaceutical Chemistry and Bioanalytics, Germany	MiV_1a Vortragend, MiV_3a, MoN_1a, Poster, Poster, Poster
Ivanović-Burmacović, Ivana	Friedrich-Alexander-University Erlangen-Nürnberg, Deutschland	Poster
Jahn, Olaf	Max-Planck-Institut für experimentelle Medizin, Göttingen, Deutschland; Center for Nanoscale Microscopy and Molecular Physiology of the Brain, 37075 Göttingen, Germany	MiV_3a, MoN_1a, Poster Vortragend
Jahnke, Siegfried	IBG-2 Pflanzenwissenschaften, Forschungszentrum Jülich, Deutschland	Poster
Jakimovska, Viktorija	Ss. Cyril and Methodius University of Skopje, Republic of Macedonia	Poster
Jakubowski, Norbert	Bundesanstalt für Materialforschung und -prüfung, Berlin	Poster

Autor(en)	Organisation(en)	Session
Janzik, Ingar	IBG-2 Pflanzenwissenschaften, Forschungszentrum Jülich, Deutschland	Poster
Jeck, Viola	Westfälische Wilhelms-Universität Münster, Deutschland	Poster Vortragend
Jeibmann, Astrid	University Hospital of Münster, Institute of Neuropathology, Münster, Germany	MoV_2a
Jertz, Roland	Bruker Daltonik GmbH, Bremen, Germany	MiV_2a, Poster
John, Harald	Bundeswehr Institute of Pharmacology and Toxicology	Poster, Poster
Jones, Emrys	Waters Corporation, United Kingdom	MoV_2b
Joseph, Shai R	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany, Deutschland	MiV_1a
Josephs, Jonathan	Thermo Fisher Scientific, USA	Poster
Jurk, Kerstin	Center for Thrombosis and Hemostasis, Universitätsklinikum der Johannes Gutenberg-Universität Mainz, Mainz, Germany;	MoN_1a
Kade, Stephanie	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	Poster
Kadesch, Patrik	Justus-Liebig-Universität Gießen, Institut für Anorganische und Analytische Chemie	MoN_2a Vortragend
Kaefer, Uwe	Cooperation Group ''Comprehensive Molecular Analytics", Helmholtz Zentrum Muenchen, Munich, GERMANY	Poster
Käfer, Uwe	Helmholtz Zentrum Muenchen, Neuherberg	MiV_2a Vortragend
Kaftan, Filip	Max Planck Institute for Chemical Ecology, Jena, Germany	Poster
Kaleja, Patrick	AG Systematische Proteomforschung & Bioanalytik, Institut für Experimentelle Medizin, Christian-Albrechts-Universität, Kiel; Klinik für Unfallchirurgie und Traumatologie, Experimentelle Unfallchirurgie, UKSH, Kiel	Poster Vortragend
Kalinowski, Jörn	Bielefeld University, Bielefeld, Deutschland	Poster
Kalkhof, Stefan	Helmholtz-Centre for Environmental research (UFZ), Department of Molecular Systems Biology, Leipzig, Germany; Coburg University, Department of Applied Sciences, Coburg, Germany	Poster, Poster
Kanawati, Basem	Helmholtz Zentrum München, Deutschland	MiV_2a Vortragend
Kappert, Christin	Max Planck Institute for Biophysical Chemistry, Göttingen, Germany	DiV_3a
Karaköse, Hande	Division of Bioanalytical Chemistry, Research Center Borstel, Germany; German Center for Infection Research, Clinical Tuberculosis Center, Borstel, Germany	Poster Vortragend
Karas, Michael	Goethe Universität, Frankfurt, Deutschland	Poster, Poster, MiV_1a, Poster
Karimi, Kudratullah	Goethe-University Frankfurt/Main, Deutschland	Poster Vortragend
Karst, Uwe	Westfälische Wilhelms-Universität Münster, Deutschland; University of Münster, Institute of Inorganic and Analytical Chemistry, Münster, Germany	DiV_2a, MoV_2a, MoV_2a, MoV_2b, MoV_4a, MoV_4a, Poster, Poster, Poster, Poster, Poster
Kaspar-Schoenefeld, Stephanie	Bruker Daltonik GmbH, Deutschland	Poster
Kasuch, Sandra	Federal Criminal Police Office, Forensic Institute, 65193 Wiesbaden, Germany	MoN_2a
Kaub, Johannes	Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Deutschland	Poster Vortragend
Kellner, Ina	Friedrich-Alexander-University Erlangen-Nürnberg, Deutschland	Poster Vortragend
Keppler, Bernhard K.	Universität Wien, Österreich	MoV_4a
Kessler, Nikolas	Bruker Daltonik GmbH, Deutschland	Poster

Autor(en)	Organisation(en)	Session
Kettling, Hans	University of Münster, Insitute for Hygiene, Münster, Germany; Interdisciplinary Center for Clinical Research (IZKF) Münster, Germany	Poster
Khalil, Saleh mahmud	Justus Liebig University Giessen, Institute of Inorganic and Analytical Chemistry	MoV_2a Vortragend
Kiani, Parnian	University Medical Centre Hamburg-Eppendorf, Institute for Clinical Chemistry, Department for Mass Spectrometric Proteomics, Hamburg	Poster Vortragend
Kim, Ahyoung	Leibniz Institute of Plant Biochemistry, Department of Bioorganic Chemistry; Universität Leipzig, Faculty of Chemistry and Mineralogy	Poster Vortragend
Kiontke, Andreas	Universität Leipzig, Deutschland	MoN_3a Vortragend
Kipping, Marc	Waters GmbH, Eschborn, Deutschland	Poster Vortragend, Poster Vortragend
Kirsch, Dieter	Federal Criminal Police Office, Forensic Institute, 65193 Wiesbaden, Germany	MoN_2a
Kivala, Milan	Friedrich-Alexander-University Erlangen-Nürnberg, Germany	DiV_1a
Klee, Sonja	TOFWERK, Schweiz	Poster Vortragend
Klein, Jonas	University Medical Center Hamburg-Eppendorf, Deutschland	Poster Vortragend
Kniese, Jasmin	Universität Bayreuth, Deutschland	Poster
Knochenmuss, Richard	Tofwerk, Uttigenstrasse 22, CH-3600 Thun, Switzerland	DiV_4a
Koch, Annika	Institute for Hygiene, University of Münster, Robert-Koch-Str. 41, 48149 Münster, Germany	Poster
Koch, Annika	University of Münster, Institute of Hygiene, Biomedical Mass Spectrometry, Germany	Poster Vortragend
Koch, Arne	University of Leipzig, Germany	Poster
Koch, Winfried	Oil-Wärme-Institut GmbH, Herzogenrath, Deutschland	Poster
Koellensperger, Gunda	Universität Wien, Österreich	MoV_4a
Koenig, Stefan	Institute of Forensic Medicine, University of Bern	Poster
Köhler, Jörg	Markes International GmbH, Schleussnerstrasse 42, Frankfurt, Germany	MoN_3a
Köhler, Niklas	Division of Clinical Infectious Diseases, Research Center Borstel, Borstel, Germany; German Center for Infection Research, Clinical Tuberculosis Center, Borstel, Germany	Poster
Kokesch-Himmelreich, Julia	Universität Bayreuth, Deutschland	Poster
Kölbel, Knut	Universiteit Antwerpen, Belgien	DiV_4a Vortragend
Kolter, Marlene	Georg-August-Universität Göttingen, Deutschland	Poster Vortragend
Komorowski, Lars	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	Poster
Kompauer, Mario	Justus Liebig University Giessen, Germany; Institut für Anorganische und Analytische Chemie; Justus-Liebig-Universität Gießen	MoV_2b Vortragend, Poster
Kondyli, Aikaterini	Max Planck Institut für Kohlenforschung, Germany	Poster Vortragend
Konietzny, Rebecca	Agilent Technologies, Waldbronn, Deutschland	DiV_4a
König, Simone	WWU Münster	MiV_1a
König, Vanessa	Hochschule Mannheim, Deutschland	Poster
Kopczynski, Dominik	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Otto-Hahn-Str. 6b, 44227 Dortmund, Germany	DiN_1a Vortragend, DiN_3a
Kopicki, Janine	Heinrich-Pette-Institut, Hamburg, Deutschland	Poster Vortragend

Autor(en)	Organisation(en)	Session
Koschinski, Stefan	Markes International GmbH, Schleussnerstrasse 42, Frankfurt, Germany	MoN_3a
Köster, Claus	Bruker-Daltonik GmbH, Bremen	Poster
Koszinowski, Konrad	Georg-August-Universität Göttingen, Deutschland	Poster, Poster, MoV_3b Vortragend, Poster, Poster, Poster
Kowol, Christian R.	Universität Wien, Österreich	MoV_4a
Kozlov, Ilya	University of Leipzig, Germany	Poster
Kraj, Agnieszka	ANTEC, Leyden	Poster
Krajewski, Matthias	Division of Bioanalytical Chemistry, Research Center Borstel, Parkallee 10, Borstel, Germany	MoV_1b
Kramer, Katharina	Max Planck Institute for Plant Breeding Research, Köln, Germany	DiV_3a
Kratochvil, Isabel	Helmholtz-Centre for Environmental research (UFZ), Department of Molecular Systems Biology, Leipzig, Germany	Poster Vortragend
Kraus, Johanna	Fort Collins Science Center, US Geological Survey, Fort Collins, USA	MoV_2b
Krause, Eberhard	Leibniz-Institut für molekulare Pharmakologie (FMP), Deutschland	MoN_1a, Poster
Kreyenschmidt, Friedrich	Georg-August-Universität Göttingen, Deutschland	MoV_3b, Poster Vortragend
Kriete, Claudia	Bruker Daltonik GmbH, Bremen, Germany	MiV_2a, Poster
Kröger, Nils	B-CUBE Center for Molecular Bioengineering, Dresden, Deutschland; Department of Chemistry and Food Chemistry, Technische Universität Dresden, Deutschland	MiV_3a
Kröger, Sabrina	University of Münster, Institute of Inorganic and Analytical Chemistry, Münster, Germany	MoV_2a Vortragend
Krösser, Dennis	University Medical Center Hamburg Eppendorf, Deutschland	Poster, Poster Vortragend
Krüger, Sascha	Universität Kiel, Deutschland	Poster
Kruth, Claudia	Universität Rostock, Deutschland	MoN_3a
Kuballa, Juergen	GALAB Laboratories GmbH, Deutschland	DiN_1a
Kuballa, Jürgen	GALAB Laboratories GmbH, Deutschland	Poster
Kuck, Dietmar	Department of Chemistry, Bielefeld University	Poster Vortragend, Poster Vortragend
Kücklich, Marlen	Universität Leipzig, Deutschland	Poster
Kugler, Christian	LungenClinic Großhansdorf, Wöhrendamm 80, 22927 Großhansdorf.	DiN_3a
Kühne, Stephan	Bruker Daltonik GmbH, Deutschland	Poster Vortragend, Poster Vortragend
Kukačka, Zdeněk	Steinbeis Center for Biopolymer Analysis and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany	Poster
Kulkarni, Purva	Max Planck Institute for Chemical Ecology, Jena, Germany; Lehrstuhl für Bioinformatik, Friedrich Schiller University, Jena, Germany; Research Group Mass spectrometry/Proteomics, Max Planck Institute for Chemical Ecology	DiN_2a, MoV_3b
Kulle, Alexandra	Universitätsklinikum Schleswig-Holstein, Deutschland	MoV_4b Vortragend
Kumar, Mukesh	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany, Deutschland	MiV_1a Vortragend
Kuo, Alex	Academia Sinica, School of Chemistry, Taipei, Taiwan	Poster
Kurulugama, Ruwan	Agilent Technologies, Santa Clara, USA	DiV_4a
Kusch, Kathrin	Department of Neurogenetics, Max-Planck-Institute of Experimental Medicine, 37075 Göttingen, Germany	Poster
Kuzmich, Oleksandra	Humboldt Universität zu Berlin, Deutschland	MoN_1a Vortragend

Autor(en)	Organisation(en)	Session
Kwiatkowski, Marcel	University Medical Center Groningen, Department of Pulmonary Diseases and Tuberculosis, Groningen, The Netherlands.; University of Groningen, Department of Analytical Biochemistry, The Netherlands.	Mo_Pr Vortragend
Kwiatkowski, Marcel	Mass Spectrometric Proteomics, Department of Clinical Chemistry, University Medical Center Hamburg-Eppendorf, Hamburg, Germany.	Poster
Lang, Johannes	II physikalisches Insitut, Justus-Liebig-Universität Gießen, Deutschland	Poster
Lange, Christoph	Division of Clinical Infectious Diseases, Research Center Borstel, Borstel, Germany; German Center for Infection Research, Clinical Tuberculosis Center, Borstel, Germany; International Health/Infectious Diseases, University of Lübeck, Lübeck, Germany	Poster
Lange, Mike	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig; Center for Biotechnology and Biomedicine, Universität Leipzig, Germany	MoV_1a
Lange, Tobias	University Medical Center Hamburg-Eppendorf, Deutschland	Poster
Langer, Julian	MPI for Biophysics, Frankfurt am Main, GERMANY	Poster
Langridge, James	Waters Corporation, Wilmslow, United Kingdom	Poster, Poster, Poster
Lebon, Alexandre	UMR CNRS 6521, Université de Bretagne Occidentale, 6 Av.Le Gorgeu, 29200 Brest, France	MoV_3a
Lee, Hee-Jin	Humboldt-Universität zu Berlin, Deutschland	Poster
Lehmann, Sylvain	Laboratoire de Biochimie et Protéomique Clinique, Institut de Médecine Régénératrice et de Biothérapie, CHU de Montpellier - Hôpital St. Eloi, Montpellier, France	Poster
Lehmann, Wolf-Dieter	Biochemie-Zentrum Heidelberg, Deutschland; DKFZ Heidelberg; Deutsches Krebsforschungszentrum (DKFZ) Heidelberg	MoV_1a, Poster Vortragend
Leipert, Jan	AG Systematische Proteomforschung & Bioanalytik, Institut für Experimentelle Medizin, Christian-Albrechts-Universität zu Kiel, Kiel, Deutschland	Poster Vortragend
Lemesheva, Valeriia	St-Petersburg State University, Russia	Poster
Lemmnitzer, Katharina	University of Leipzig, Medical Faculty, Institute of Medical Physics and Biophysics	DiV_4a Vortragend
Lenz, Thomas	caprotec bioanalytics GmbH	MoN_1a
Leonhard, Peter	Merck KGaA, Frankfurter Str. 250, 64293 Darmstadt, Germany	Poster
Leveridge, Melanie	Departments of Platform Technology & Science, GlaxoSmithKline, Stevenage, UK	Poster
Lewin, Yannik	Goethe Universität, Frankfurt, Deutschland	Poster Vortragend
Li, Bin	Department of Chemistry, University of Illinois, 405 North Mathews Avenue, 61801 Urbana, Illinois, USA	DiV_2a
Li, Liang	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster
Li, Yan	Helmholtz Zentrum München, Deutschland	MiV_2a
Li, Zhendong	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster, Poster
Lieblein, Tobias	Goethe-Universität Frankfurt, Deutschland	MiV_3a Vortragend
Liepold, Thomas	Proteomics Group, Max-Planck-Institute of Experimental Medicine, 37075 Göttingen, Germany	Poster

Autor(en)	Organisation(en)	Session
Linke, Dennis	Div. Systematic Proteome Research & Bioanalytics, Institute for Experimental Medicine, Kiel University, Germany	Poster
Linscheid, Michael	Humboldt-Universität zu Berlin	Poster, MoN_1a
Linscheid, Michael W.	Humboldt-Universität zu Berlin, Institut für Chemie, Deutschland	Poster, Poster, Poster
Lippert, Wayne	II physikalisches Insitut, Justus-Liebig-Universität Gießen, Deutschland	Poster
Liu, Fan	Universiteit Utrecht, The Netherlands	Poster
Lockhauserbäumer, Julia	Heinrich-Pette-Institute Leibniz Institute for Experimental Virology, Deutschland	Poster
Löhmannsröben, Hans-Gerd	University of Potsdam, Germany	Poster
Lopez, Javier	Bruker Espanola S.A., Madrid, Spanien	Poster
Lopez-Hilfiker, Felipe	TOFWERK, Schweiz; Paul Scherrer Institute (PSI), Villigen, Switzerland	Poster
Lorenz, Jana	1Department of Pharmaceutical Chemistry and Bioanalytics, Institute of Pharmacy, Martin-Luther University Halle-Wittenberg, Halle (Saale), Germany	Poster Vortragend
Lorenz, Yvonne	Universität Bonn, Deutschland	Poster Vortragend
Loroch, Stefan	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Deutschland	MoN_1a, MoV_4b Vortragend
Lotz, Florian	Justus-Liebig-Universität Gießen, Deutschland	MiV_2a Vortragend
Lubeck, Markus	Bruker Daltonik GmbH, Deutschland	Poster
Luckau, Luise	Physikalisch-Technische-Bundesanstalt, Deutschland	Poster Vortragend
Luetjohann, Jens	GALAB Laboratories GmbH, Deutschland	DiN_1a Vortragend
Luginbühl, Marc	Institute of Forensic Medicine, University of Bern	Poster Vortragend
Lukasheva, Elena	Universität St. Petersburg, Lehrstuhl Biochemie, Russia	DiV_3a
Luo, Ruoji	Max-Planck-Institut für Kohlenforschung, Deutschland	Poster Vortragend
Luo, Xian	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster
Lupu, Loredana	Steinbeis Center for Biopolymer Analysis and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany; Proteome Center, Institute of Immunology, University of Rostock, Rostock, Germany	Poster
Lützen, Elias	Westfählische Wilhelms-Universität Münster	Poster Vortragend
Maeser, Stefan	Steinbeis Center for Biopolymer Analysis and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany	Poster
Mairinger, Teresa	BOKU Wien, Österreich	DiV_4a
Makowski, Marcus R.	Charité, Berlin	Poster
Mallagaray, Alvaro	Institute of Chemistry, University of Lübeck, Lübeck, Germany	Poster
Mannaa, Atef	Mass Spectrometric Proteomics, Department of Clinical Chemistry, University Medical Center Hamburg-Eppendorf, Hamburg, Germany.	Poster Vortragend
Manns, Annika	Leibniz Institut für Molekulare Pharmakologie, Deutschland	Poster Vortragend
Marcillo, Andrea	University of Leipzig, Germany	Poster Vortragend, Poster
Marella, Chakravarthy	Research Center Borstel, Division of Bioanalytical Chemistry, Parkallee 1-40, D-23845 Borstel, Germany.	DiN_3a
Marianski, Mateusz	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland	MiV_2a
Marshall, Peter	Departments of Platform Technology & Science, GlaxoSmithKline, Stevenage, UK	Poster
Martin, Diego	Bruker Espanola S.A., Madrid, Spanien	Poster

Autor(en)	Organisation(en)	Session
Massolini, Gabriella	Department of Drug Sciences, University of Pavia, Pavia, Italy	Poster
Matamoros, Manuel	Estación Experimental de Aula Dei, Consejo Superior de Investigaciones Científicas (CSIC), Department of Plant Nutrition	Poster
Matsubara, Shizue	IBG-2 Pflanzenwissenschaften, Forschungszentrum Jülich, Deutschland	Poster
Mattheij, Nadine J.	Department of Biochemistry, Cardiovascular Research Institute Maastricht, Maastricht University, The Netherlands;	MoN_1a
Mävers, Stephan	Bruker Daltonik GmbH, Deutschland	Poster
May, Jody	Vanderbilt University, USA	DiV_4a
Mazzone, Massimiliano	Laboratory of Molecular Oncology and Angiogenesis, Vesalius Research Center, Leuven, Belgium	MoV_4b
McGregor, Laura	Markes International, Gwaun Elai Medi-Science Campus, Llantrisant, RCT, Wales, United Kingdom	MoN_3a
McLean, John	Vanderbilt University, USA	DiV_4a
McLean, Lynn	Centre for Proteome Research, Institute of Integrative Biology, University of Liverpool, Liverpool, UK	Poster
Meckenstock, Rainer U.	Bio-film Center Universität Duisburg-Essen	Poster
Medvedev, Sergei	Department of Plant Physiology and Biochemistry, St. Petersburg State University	Poster, Poster
Mehmood, Tahir	Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry, Germany	Poster
Meijers, Rob	European Molecular Biology Laboratory (EMBL), Hamburg, Germany	MiV_3a
Meiler, Jens	Vanderbilt University, Nashville, Tennessee, USA	MoN_1a
Meinhardt, Ute	Friedrich-Alexander-University Erlangen-Nürnberg, Germany	DiV_1a
Melzig, Matthias F.	Freie Universität Berlin, Institute of Pharmacy, Pharmaceutical Biology	Poster
Memboeuf, Antony	UMR CNRS 6521, Université de Bretagne Occidentale, 6 Av.Le Gorgeu, 29200 Brest, France	MoV_3a
Menezes, Riya Christina	Max Planck Institute for Chemical Ecology, Jena, Germany	DiN_2a Vortragend
Mercanoglu, Baris	University Medical Center Hamburg Eppendorf, Deutschland	Poster
Meyer, Bernd	Uni Hamburg, Deutschland	Poster
Meyer, Nele	University of Bonn	Poster
Meyer, Stefanie	Friedrich Schiller University Jena, Deutschland	MoN_2a
Meyer, Sven W.	Bruker Daltonik GmbH, Deutschland	Poster
Michaelis, Simon	caprotec bioanalytics GmbH	MoN_1a
Michalski, Annette	Bruker Daltonik GmbH, Deutschland	Poster
Michalzik, Beate	Friedrich Schiller University Jena, Deutschland	MoN_2a
Milentyev, Alexander	MPI-CBG, Dresden, Deutschland	MiV_3a Vortragend
Milkovska-Stamenova, Sanja	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig; Center for Biotechnology and Biomedicine, Universität Leipzig	MoV_4a Vortragend
Miller, Dwayne	Max Planck Institute for the Structure and Dynamics of Matter	Poster, Poster
Miller, Janet	Fort Collins Science Center, US Geological Survey, Fort Collins, USA	MoV_2b
Miller, R. J. Dwayne	Max Planck Institute for the Structure and Dynamics of Matter, Atomically Resolved Dynamics Division, Luruper Chaussee 149,	Poster, Poster, Poster

Autor(en)	Organisation(en)	Session
	22761 Hamburg, Germany.; Max Planck Institut für Struktur und Dynamik der Materie, Hamburg, Deutschland; Department of Chemistry and Physics, University of Toronto, Toronto, Canada	
Milrud, Svetlana	Department of Plant Physiology and Biochemistry, St. Petersburg State University, Russia; Department of Biochemistry, St. Petersburg State University, Russia	DiV_3a
Minameyer, Martin B.	Friedrich-Alexander-University Erlangen-Nürnberg, Germany	Poster, DiV_1a Vortragend
Mindukshev, Igor	Sechenov Institute of Evolutionary Physiology and Biochemistry, Russian Academy of Sciences, Saint Petersburg, Russia;	MoN_1a
Mischnick, Petra	Technische Universität Braunschweig, Deutschland	Poster
Miske, Ramona	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	Poster
Mitrofanov, Elena	Christian-Albrechts-Universität, Deutschland	Poster Vortragend
Mnatsakanyan, Ruzanna	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig; Center for Biotechnology and Biomedicine, Universität Leipzig	MoV_4a
Möbius, Wiebke	Department of Neurogenetics, Max-Planck-Institute of Experimental Medicine, 37075 Göttingen, Germany; Center for Nanoscale Microscopy and Molecular Physiology of the Brain, 37075 Göttingen, Germany	Poster
Mock, Hans-Peter	IPK-Gatersleben, Deutschland	Poster
Moise, Adrian	Department of Chemistry, University of Konstanz, Konstanz, Germany	Poster
Mokhtar, Mohamed	Christian-Albrechts-Universität zu Kiel, Deutschland	Poster
Möller, Manfred	Uniklinik der RWTH Aachen, Deutschland	Poster
Möller, Stephanie	Biomaterials Department, INNOVENT e.V., Jena, Germany	Poster
Mordehai, Alex	Agilent Technologies, Santa Clara, USA	DiV_4a
Morgner, Nina	Goethe-Universität Frankfurt, Deutschland; Institut für Physikalische und Theoretische Chemie, Goethe-Universität Frankfurt	MiV_3a, MiV_3a, Poster, Poster, Poster, Poster
Mormann, Michael	Institut für Hygiene, Universität Münster, Deutschland	Poster, Poster
Morrice, Nick	SCIEX, UK	Poster
Mucek, Katharina	Bioanalytical Mass Spectrometry, Max Planck Institute for Biophysical Chemistry, Göttingen, Germany	Poster Vortragend
Mucha, Eike	Freie Universität Berlin, Deutschland; Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland	MiV_2a
Mueller, Jennifer-Christin	Institute of Inorganic and Analytical Chemistry, University of Muenster, Corrensstr. 28/30, 48149 Muenster, Germany	Poster Vortragend
Mueller, Max A.	Justus Liebig University Giessen, Germany	MoV_2b
Mülbaier, Marcel	Cellzome GmbH, Heidelberg	MoN_1a
Müller, Julia	Pathology of the University Hospital of Lübeck and the Research Center Borstel, Clinical and Experimental Pathology, 23538 Lübeck and 23845 Borstel, Germany.	DiN_3a
Müller, Katrin	Cellzome GmbH, Heidelberg	MoN_1a
Müller, Mathias	Thermo Fisher Scientific, Bremen, Germany	Poster Vortragend

Autor(en)	Organisation(en)	Session
Müller, Miriam J.	Universität des Saarlandes, Saarbrücken, Deutschland; Saarland University, Deutschland	MoV_4b, DiV_2a Vortragend
Müller, Volker	Johann Wolfgang Goethe-Universität, Deutschland	Poster
Mung, Dorothea	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster
Muñoz-Fontela, Cesar	Heinrich-Pette-Institut, Hamburg, Deutschland	Poster
Münster-Müller, Sascha	Bundeskriminalamt Wiesbaden	Poster
Muskat, Tassilo	Christian-Albrechts-Universität, Deutschland	Poster
Näthe, Kerstin	Friedrich Schiller University Jena, Deutschland	MoN_2a
Neese, Stephan	Justus-Liebig-Univeristät Gießen, Deutschland	Poster
Neubauer, Lisa	Institute of Plant Biology and Biotechnology, University of Münster, Germany	Poster
Neugebauer, Thomas	Friedrich-Alexander-University Erlangen-Nürnberg, Deutschland	Poster Vortragend
Neumann, Anika	Joint Mass Spectrometry Centre / Chair of Analytical Chemistry, University of Rostock, 18059 Rostock, Germany	MoN_2a, Poster Vortragend
Neumann, Heinz	Free Floater (Junior) Research Group Applied Synthetic Biology, Georg-August University Göttingen, Institute for Microbiology and Genetics, 37077 Göttingen, Germany	Poster
Neupärtl, Moritz	Goethe-Universität-Frankfurt	MiV_1a
Neuweger, Heiko	Bruker Daltonik GmbH, Deutschland	Poster, Poster
Neuwohner, Andrea	IBG-2 Pflanzenwissenschaften, Forschungszentrum Jülich, Deutschland	Poster
Nguyen, Minh	ISAS, Deutschland	MiV_1a
Ni, Zhixu	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig; Center for Biotechnology and Biomedicine, Universität Leipzig, Germany	MoV_1a
NicDaeid, Niamh	University of Dundee, CAHID, School of Science and Engineering, Dundee, DD15EH, Scotland	MoN_2a
Niehoff, Ann-Christin	University of Münster, Institute of Inorganic and Analytical Chemistry, Münster, Germany	MoV_2a
Nikolaev, Eugene N.	Institute for Energy Problems of Chemical Physics, Russian Academy of Sciences, Moscow, Russia	Poster, MiV_2a
O'Hair, Richard	University of Melbourne, Australia	Poster
Oefner, Peter J.	University of Regensburg, Institute of Functional Genomics, Regensburg, Deutschland	Poster
Opuni, Kwabena F.M.	Proteome Center Rostock, Deutschland	DiV_4a
Oster, M.	2Joint Mass Spectrometry Centre Helmholtz-Zentrum München, Comprehensive Molecular Analytics (CMA), Neuherberg, Germany	Poster
Othman, Alaa	University of Lübeck, Germany	DiV_2a
O'Hair, Richard A. J.	The University of Melbourne, Australia	Plenarvortrag 3 Vortragend
Pagel, Kevin	Freie Universität Berlin; Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin; Fritz-Haber-Institut Berlin, Deutschland	DiV_4a, MiV_2a Vortragend, MiV_3a, Poster
Papan, Cyrus	SCIEX GmbH, Darmstadt, GERMANY	Poster Vortragend
Parchomyk, Tobias	Georg-August-Universität Göttingen, Deutschland	Poster Vortragend
Passig, Johannes	Universität Rostock, Deutschland; Joint Mass Spectrometry Centre University	MoN_3a, Poster Vortragend

Autor(en)	Organisation(en)	Session
	of Rostock, Chair of Analytical Chemistry, Rostock, Germany	
Paudel, Gagan	Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry (Halle/Saale); Faculty of Chemistry and Mineralogy, Universität Leipzig	DiV_3a
Paudyal, Bhesh Raj	Department of Cellular Microbiology, Research Center Borstel, Parkallee 22, Borstel, Germany	MoV_1b
Peetz, Oliver	University of Frankfurt, Deutschland	MiV_3a Vortragend
Peng, Bing	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Germany	DiN_3a Vortragend
Penkert, Martin	Leibniz-Institut für molekulare Pharmakologie (FMP), Deutschland; Humboldt-Universität zu Berlin	MoN_1a Vortragend
Penner, Alexander	Justus-Liebig-Univeristät Gießen, Deutschland	Poster
Perez, Cesar	Bruker Espanola S.A., Madrid, Spanien	Poster
Persicke, Marcus	Bielefeld University, Bielefeld, Deutschland	Poster
Peters, Thomas	Institute of Chemistry, University of Lübeck, Lübeck, Germany	Poster
Pietschke, Cleo	Zoologisches Institut, Uni Kiel	Poster
Pikhtelev, Alexander	Institute of Energy Problems of Chemical Physics, Russian Academy of Sciences, Russia	Poster
Piotrowski, Christine	Martin-Luther-Universität Halle-Wittenberg, Deutschland	MoN_1a Vortragend
Planitz, Peter	Agilent Technologies, Waldbronn, Germany	MoV_4a
Plaß, Wolfgang R.	II physikalisches Insitut, Justus-Liebig-Universität Gießen, Deutschland; GSI Darmstadt, Deutschland	Poster
Poeckel, Daniel	Cellzome GmbH, Heidelberg	MoN_1a
Pogan, Ronja	Heinrich-Pette-Institute Leibniz Institute for Experimental Virology, Deutschland	Poster Vortragend
Pohlentz, Gottfried	Institut für Hygiene, Universität Münster, Deutschland	Poster Vortragend
Popkova, Yulia	Leipzig University, Faculty of Medicine, Institute for Medical Physics and Biophysics, Germany	MoV_3b Vortragend
Pospilova, Veronika	Paul Scherrer Institute (PSI), Villigen, Switzerland	Poster
Potthoff, Alexander	Institute for Hygiene, University of Münster, Robert-Koch-Str. 41, 48149 Münster, Germany	Poster Vortragend
Pötz, Oliver	Natural and Medical Sciences Institute at the University of Tübingen, Tübingen, Germany;	MoN_1a
Poulsen, Nicole	B-CUBE Center for Molecular Bioengineering, Dresden, Deutschland	MiV_3a
Prasse, Daniela	Institute for General Microbiology, Kiel University, Germany	Poster
Probst, Christian	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	Poster
Przybylski, Michael	Steinbeis Center for Biopolymer Analysis and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany	Poster, Poster
Pütz, Michael	Bundeskriminalamt Wiesbaden	Poster
Quack, Thomas	Justus-Liebig-Universität Gießen, Institut für Parasitologie	MoN_2a
Rabe, Klaus F.	LungenClinic Großhansdorf, Wöhrendamm 80, 22927 Großhansdorf.; Airway Research Center North, German Center for Lung Research, Wöhrendamm 80, 22927 Großhansdorf, Germany	DiN_3a
Raja, Erum	Thermo Fisher Scientific, Rockford, IL, USA	Poster
Raupers, Björn	Universität Kiel, Deutschland	Poster Vortragend

Autor(en)	Organisation(en)	Session
Rehkamp, Anne	Martin-Luther-University Halle-Wittenberg, Institute of Pharmacy, Department of Pharmaceutical Chemistry and Bioanalytics, Germany	Poster Vortragend
Reinert, Thorben	Christian-Albrechts-Universität zu Kiel, Deutschland	Poster Vortragend
Renné, Thomas	University Medical Center Hamburg Eppendorf, Deutschland	MiV_1a
Rennie, Emma	Agilent Technologies, Santa Clara, USA	DiV_4a
Reuter, Jörn Hendrik	Research and Development, Beiersdorf AG, Hamburg	Poster
Richardson, Keith	Waters Corporation, Wilmslow, United Kingdom	Poster, Poster
Riebe, Daniel	University of Potsdam, Germany	Poster
Riedel, Jens	Bundesanstalt für Materialforschung- und prüfung, Deutschland	Poster, Poster, Poster
Riemer, Thomas	University of Leipzig, Medical Faculty, Institute of Medical Physics and Biophysics	DiV_4a
Rinaldi, Francesca	Department of Drug Sciences, University of Pavia, Pavia, Italy	Poster Vortragend
Rissanen, Kari	Department of Chemistry, NanoScience Center, University of Jyvaskyla, Finnland	DiV_4a
Robertson, Wesley D.	Max Planck Institut für Struktur und Dynamik der Materie, Hamburg, Deutschland	Poster, Poster
Röcken, Christoph	Institute of Pathology, Christian-Albrechts-Universität, Kiel, Germany	MoV_4b
Roeck, Walter	Bruker BioSpin AG, Fällanden, Switzerland	MiV_2a
Rohn, Sascha	Universität Hamburg, Grindelallee 117, Hamburg; Universität Hamburg, Deutschland	Poster, Poster
Rohner, Urs	TOFWERK, Switzerland	Poster Vortragend
Romanovskaya, Ekaterina	Department of Biochemistry, St. Petersburg State University, Russia	Poster
Römpp, Andreas	Department of Food Analysis, University of Bayreuth, E.-C.-Baumann-Str. 20, 95326 Kulmbach, Bayreuth, Germany; Chair of Bioanalytical Sciences and Food Analysis, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth, Germany; Universität Bayreuth, Deutschland	DiV_2a, MoV_2b Vortragend, Poster, Poster
Roth, Alexander	Hochschule Mannheim, Deutschland	Poster Vortragend
Rüger, Christopher Paul	University of Rostock, Rostock; Joint Mass Spectrometry Centre / Chair of Analytical Chemistry, University of Rostock, 18059 Rostock, Germany	MiV_2a, Poster, MoN_2a Vortragend
Rühl, Michael	Goethe-Universität Frankfurt am Main, Deutschland	Poster Vortragend, Poster
Rurack, Knut	Bundesanstalt für Materialforschung und -prüfung	Poster
Rutjens, Sofie	Laboratory of Toxicology, University of Ghent	Poster
Rychlik, Michael	Technische Universität Münschen, Lehrstuhl für Analytische Lebensmittelchemie	Poster
Saluz, Hans Peter	Department Cell and Molecular Biology, Leibniz Institute for Natural Product Research and Infection Biology	MoV_3b
Sanchez-Carballo, Patricia	Division of Clinical Infectious Diseases, Research Center Borstel, Borstel, Germany; German Center for Infection Research, Clinical Tuberculosis Center, Borstel, Germany	Poster
Satilmis, Ilker	Max-Planck-Institut für Kohlenforschung, Deutschland	Poster Vortragend
Sauerland, Volker	Bruker Daltonik GmbH, Germany	Poster

Autor(en)	Organisation(en)	Session
Savitski, Mikhail M.	Cellzome GmbH, Heidelberg; EMBL, Heidelberg	MoN_1a
Sawers, Gary	2Department of Microbiology, Institute of Biology, Martin-Luther University Halle-Wittenberg, Halle (Saale), Germany	Poster
Schachel, Tilo D.	Westfälische Wilhelms-Universität Münster, Deutschland	Poster Vortragend
Schade, Julian	Joint Mass Spectrometry Centre University of Rostock, Chair of Analytical Chemistry, Rostock, Germany	Poster
Schäfer, Frank	Federal Criminal Police Office, Forensic Institute, 65193 Wiesbaden, Germany	MoN_2a
Schäfer, Mathias	Institute for Organic Chemistry, Department of Chemistry, University of Cologne; Universität zu Köln, Deutschland	MiV_1a, Poster, DiV_1a
Schäfer, Mathias	Institute of Organic Chemistry, University of Cologne, Greinstraße 4, 50939 Köln, Germany	MoV_1b
Schaible, Ulrich E.	Department of Cellular Microbiology, Research Center Borstel, Parkallee 22, Borstel, Germany	MoV_1b
Schalley, Christoph A.	Freie Universität Berlin	DiV_4a
Scharf, Madeleine	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	Poster
Scharrenbroch, Lisa	Federal Criminal Police Office, Forensic Institute, 65193 Wiesbaden, Germany; University of Dundee, CAHID, School of Science and Engineering, Dundee, DD15EH, Scotland	MoN_2a Vortragend
Schatz, Jürgen	Friedrich-Alexander-University Erlangen-Nürnberg, Germany	DiV_1a
Scheeren, Simon Gereon	Westfälische Wilhelms-Universität Münster, Deutschland	DiV_2a Vortragend
Scheffler, Kai	Thermo Fisher Scientific, Deutschland	Poster, Poster
Scheidegger, Oliver	Hoffmann la Roche AG, Schweiz	Poster
Scheidenberger, Christoph	II physikalisches Insitut, Justus-Liebig-Universität Gießen, Deutschland; GSI Darmstadt, Deutschland	Poster
Scheier, Rico	Universität Bayreuth, Deutschland	Poster
Schelhaas, Mario	Institute of Molecular Virology & Institute of Medical Biochemistry Münster, WW University of Münster, Germany	Poster
Schenk, Regina	Humboldt-Universität zu Berlin, Albrecht Daniel Thaer-Institute for Crop Science	Poster
Schiller, Jürgen	University of Leipzig, Medical Faculty, Institute of Medical Physics and Biophysics	DiV_4a, MoV_3b
Schilyaev, Nikita	Universität St. Petersburg, Lehrstuhl Biochemie, Russia	DiV_3a
Schlichting, Rita	Helmholtz-Centre for Environmental research (UFZ), Department of Cell Toxicology, Leipzig, Germany	Poster
Schlüter, Hartmut	University Medical Center Hamburg-Eppendorf, Deutschland	DiN_1a, Poster
Schlüter, Hartmut	Universitätsklinikum Hamburg-Eppendorf, Germany; University Medical Center Hamburg Eppendorf, Deutschland; Mass Spectrometric Proteomics, Department of Clinical Chemistry, University Medical Center Hamburg-Eppendorf, Hamburg, Germany.; University Medical Centre Hamburg-Eppendorf, Institute of Clinical Chemistry, Department for Mass Spectrometric Proteomics, Hamburg Germany	DiV_3a, MiV_1a, Poster, Poster, Poster, Poster, Poster
Schmid, Robin	Institute of Food Chemistry, University of Münster, Germany;	Poster Vortragend

Autor(en)	Organisation(en)	Session
	Institute of Inorganic and Analytical Chemistry, University of Münster, Germany	
Schmidt, Carla	Interdisciplinary research center HALOmem, Martin Luther University University Halle-Wittenberg	MoN_1a Vortragend, Poster, MoV_1a
Schmidt, Charlie	PerkinElmer LAS (Germany) GmbH, Deutschland	Poster
Schmidt, Heinar	Universität Bayreuth, Deutschland	Poster
Schmidt, Johannes R.	Department for Molecular Systems Biology, Helmholtz Centre for Environmental Research – UFZ, Leipzig, Germany	Poster Vortragend
Schmidt, Rico	Institute of Pharmacy, Martin-Luther Universität Halle-Wittenberg	DiV_3a, Poster
Schmidt, Travis	Fort Collins Science Center, US Geological Survey, Fort Collins, USA	MoV_2b
Schmit, Pierre-Olivier	Bruker Daltonik GmbH, Deutschland; Bruker Daltonique Wissembourg, France	Poster, Poster
Schmitt-Kopplin, Philippe	Helmholtz Zentrum München, Deutschland; Technische Universität München	MiV_2a
Schmitz, Ruth A.	Institute for General Microbiology, Kiel University, Germany	Poster
Schnapp, Andreas	Institute for Hygiene, Biomedical Mass Spectrometry, University of Münster, Germany; Institute for Hygiene, University of Münster, Robert-Koch-Str. 41, 48149 Münster, Germany	Poster, Poster
Schöllkopf, Wieland	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland	MiV_2a
Scholz, Verena	Research Center Borstel, Division of Bioanalytical Chemistry, Parkallee 1-40, D-23845 Borstel, Germany.	DiN_3a
Schönborn, Stefan	Goethe-Universität Frankfurt am Main, Deutschland	Poster
Schrader, Wolfgang	Max-Planck-Institut für Kohlenforschung, Deutschland	MiV_2a, Poster, Poster, Poster, Poster, MoV_3a, Poster
Schriewer, Alexander	WWU Münster, Deutschland	DiV_2a Vortragend
Schubert, Ulrich S.	Friedrich Schiller University Jena, Deutschland	MoN_2a
Schuhmann, Kai	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Deutschland	DiV_3a Vortragend, MoV_1b
Schulz, Sabine	Justus-Liebig-Universität Gießen, Deutschland	MiV_2a, Poster
Schümann, Michael	Leibniz-Institut für molekulare Pharmakologie (FMP), Deutschland	MoN_1a, Poster
Schütze, Johannes	IPK-Gatersleben, Deutschland	Poster Vortragend
Schwaiger-Hufnagel, Ulrike	Bruker Daltonik GmbH, Bremen, Germany	Poster
Schwemer, Theo	Joint Mass Spectrometry Centre / Chair of Analytical Chemistry, University of Rostock, 18059 Rostock, Germany; HICE - Helmholtz Virtual of Complex Molecular Systems in Environmental Health – Aerosols and Health, www.hice-vi.eu	MoN_2a
Schwudke, Dominik	Research Center Borstel, Division of Bioanalytical Chemistry, Parkallee 1-40, D-23845 Borstel, Germany.; Airway Research Center North, German Center for Lung Research, Wöhrendamm 80, 22927 Großhansdorf, Germany; Division of Bioanalytical Chemistry, Research Center Borstel, Germany; German Center for Infection Research, Clinical Tuberculosis Center, Borstel, Germany	DiN_3a, MoV_1b, Poster, Poster
Seeberger, Peter	Freie Universität Berlin, Deutschland; Max-Planck-Institut für Kolloid- und	MiV_2a

Autor(en)	Organisation(en)	Session
	Grenzflächenforschung, Potsdam, Deutschland	
Seulen, Sarah	Christian-Albrechts-Universität zu Kiel, Deutschland	DiV_1a Vortragend
Shadyro, Oleg	Belarusian State University, Department of Chemistry, Leningradskaya 14, 220006, Minsk, Belarus	DiN_3a
Shema, Gerta	ISAS, Deutschland	MiV_1a
Shevchenko, Andrej	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Deutschland; MPI-CBG, Dresden, Deutschland	DiV_3a, MiV_1a, MiV_3a, MoV_1b, Plenarvortrag 5 Vortragend, Poster
Shevchenko, Anna	MPI of Cell Biology and Genetics, Dresden, Germany	Poster
Shilyaev, Nikita	Department of Biochemistry, St. Petersburg State University, Russia	DiV_3a
Sickmann, Albert	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Deutschland; Department of Chemistry, College of Physical Sciences, University of Aberdeen, United Kingdom; Medizinisches Proteom Center, Ruhr Universität Bochum, Germany	MoN_1a Vortragend, MoV_4b
Siegert, Markus	Department of Chemistry, Humboldt Universität zu Berlin, Berlin, Germany	Poster Vortragend
Siemers, Adrian	Analytik Jena AG, Jena, Germany	Poster
Simon, Fabian	Hochschule Mannheim, Deutschland	Poster
Sinz, Andrea	Martin-Luther-Universität Halle-Wittenberg, Deutschland; Institute of Pharmacy, Martin Luther University Halle-Wittenberg; Martin-Luther-University Halle-Wittenberg, Institute of Pharmacy, Department of Pharmaceutical Chemistry and Bioanalytics, Germany; 1Department of Pharmaceutical Chemistry and Bioanalytics, Institute of Pharmacy, Martin-Luther University Halle-Wittenberg, Halle (Saale), Germany	DiV_1a, DiV_3a, MiV_1a, MiV_3a, MoN_1a, Poster, Poster, Poster, Poster, Poster
Sklorz, Martin	Joint Mass Spectrometry Centre / Chair of Analytical Chemistry, University of Rostock, 18059 Rostock, Germany; Universität Rostock, Deutschland	MoN_2a, MoN_3a, Poster, Poster
Slowik, Jay	Paul Scherrer Institute (PSI), Villigen, Switzerland	Poster
Smolikova, Galina	Department of Plant Physiology and Biochemistry, St. Petersburg State University, Russia	DiV_3a, Poster, Poster
Soboleva, Alena	Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry, Germany; Department of Biochemistry, St. Petersburg State University, Russia	Poster
Sobott, Frank	Universiteit Antwerpen, Belgien	DiV_4a
Solari, Fiorella A.	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Deutschland	MoN_1a
Soltwisch, Jens	Institute for Hygiene, Biomedical Mass Spectrometry, University of Münster, Germany; Interdisciplinary Center for Clinical Research (IZKF), University of Münster, Germany; University of Münster, Insitute for Hygiene, Münster, Germany; Institute for Hygiene, University of Münster, Robert-Koch-Str. 41, 48149 Münster, Germany	MoV_3b, Poster, Poster Vortragend, Poster, Poster, Poster
Spengler, Bernhard	Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, Heinrich-Buff-Ring 17, 35392 Giessen, Germany;	DiV_2a, MiV_2a, MoN_2a, MoN_2a, MoN_3a, MoV_1b, MoV_2a, MoV_2b, Poster, Poster, Poster, Poster

Autor(en)	Organisation(en)	Session
	Justus-Liebig-Universität Gießen, Deutschland; Justus-Liebig-Universität Gießen, Institut für Anorganische und Analytische Chemie; Institut für Anorganische und Analytische Chemie; Justus-Liebig-Universität Gießen	
Sperling, Michael	Westfälische Wilhelms-Universität Münster; European Virtual Institute for Speciation Analysis; Institute of Inorganic and Analytical Chemistry, University of Münster, Münster, Germany	MoV_2a, MoV_4a
Spiteller, Peter	Universität Bremen, Deutschland	Poster
Springer, Andreas	Freie Universität Berlin, Institute of Chemistry and Biochemistry, Core Facility BioSupraMol	Poster
Stafford, George	Agilent Technologies, Santa Clara, USA	DiV_4a
Stark, Tina	Goethe-Universität Frankfurt, Deutschland	MiV_3a
Steffen, Bernhard	Forschungszentrum Jülich, Deutschland	Poster
Steffen, Pascal	University Medical Center Hamburg-Eppendorf, Deutschland	DiN_1a Vortragend, Poster, Poster
Stephanowitz, Heike	Leibniz Institut für Molekulare Pharmakologie, Deutschland	Poster
Stöcker, Winfried	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	Poster
Stokes, Caroline	Universitätsklinikum des Saarlandes, Homburg, Deutschland	MoV_4b
Stow, Sarah	Vanderbilt University, USA	DiV_4a
Streibel, Thorsten	Universität Rostock, Deutschland; Helmholtz-Zentrum München,Deutschland	Poster
Striegel, Lisa	Technische Universität Münschen, Lehrstuhl für Analytische Lebensmittelchemie	Poster
Struwe, Weston B.	Oxford Glycobiology Institute, Universität Oxford, Oxford, UK	MiV_2a
Stummer, Walter	University Hospital of Münster, Department of Neurosurgery, Münster, Germany	MoV_2a
Sturm, Patrick	TOFWERK, Switzerland	Poster
Stützer, Alexandra	Max Planck Institute for Biophysical Chemistry, Göttingen, Germany	DiV_3a Vortragend, Poster
Suckau, Detlev	Bruker Daltonik GmbH, Deutschland	DiN_2a Vortragend
Süß, Rosmarie	University of Leipzig, Medical Faculty, Institute of Medical Physics and Biophysics	DiV_4a
Sutton, Jennifer	Thermo Fisher Scientific, USA	Poster
Svatoš, Aleš	Max Planck Institute for Chemical Ecology, Jena, Germany; Research Group Mass spectrometry/Proteomics, Max Planck Institute for Chemical Ecology; Institute of Organic Chemistry and Biochemistry, AS CR, Prague, Czech Republic	DiN_2a, MoV_3b, Poster
Szesny, Matthias	Bruker Daltonik GmbH, Deutschland	DiN_2a Vortragend, Poster Vortragend, Poster Vortragend, Poster Vortragend
Tampé, Robert	Johann Wolfgang Goethe-Universität, Deutschland	Poster
Tanner, Martin	TOFWERK, Switzerland	Poster
Tarakhovskaya, Elena	Department of Plant Physiology and Biochemistry, St. Petersburg State University, Russia; St-Petersburg State University, Russia	DiV_3a, Poster Vortragend
Tatlay, Jaspaul	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster
Teegen, Bianca	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	Poster

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Temporini, Caterina	Department of Drug Sciences, University of Pavia, Pavia, Italy	Poster
Tengattini, Sara	Department of Drug Sciences, University of Pavia, Pavia, Italy	Poster
Thiele, Björn	IBG-2 Pflanzenwissenschaften, Forschungszentrum Jülich, Deutschland	Poster Vortragend
Thiermann, Horst	Bundeswehr Institute of Pharmacology and Toxicology	Poster, Poster
Thiesen, Hans-Jürgen	Institute of Immunology, University of Rostock, Germany	DiV_4a
Tholey, Andreas	Systematic Proteome Research & Bioanalytics, Institute of Experimental Medicine, Christian-Albrechts-Universität, Kiel, Germany; Christian-Albrechts-Universität zu Kiel, Deutschland; Institut für Experimentelle Medizin, Uni Kiel	MoV_4b, Poster, Poster, Poster, Poster, Poster
Thomas, Daniel A.	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland	MiV_2a
Thomas, Henrik	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Deutschland	DiV_3a, Poster
Thompson, Christopher	Bruker Daltonics, Billerica, MA, USA	Poster
Thompson, Christopher J.	Bruker Daltonics Inc., Billerica, MA, USA	MiV_2a
Tissier, Alain	Department of Cell and Metabolic Biology, Leibniz Institute of Plant Biochemistry (Halle/Saale)	DiV_3a
Torres, Tomás	Universidad Autónoma de Madrid, Spain; Instituto Madrileño de Estudios Avanzados (IMDEA)-Nanociencia, Spain	Poster
Totzeck, Matthias	University Hospital Essen, Medical Faculty, West German Heart and Vascular Center, Department of Cardiology and Department of Angiology, Germany	Poster
Towers, Mark	Waters Corporation, United Kingdom	MoV_2b
Traikov, Sofia	MPI of Cell Biology and Genetics, Dresden, Germany	Poster Vortragend
Treitz, Christian	AG Systematische Proteomforschung & Bioanalytik, Institut für Experimentelle Medizin, Christian-Albrechts-Universität zu Kiel, Kiel, Deutschland; Institut für Experimentelle Medizin, Uni Kiel	Poster, Poster Vortragend
Treu, Axel	Universität Bayreuth, Deutschland	Poster Vortragend, Poster
Trog, Sabrina	Humboldt-Universität zu Berlin, Deutschland	Poster Vortragend
Tudzynski, Paul	Institute of Plant Biology and Biotechnology, University of Münster, Germany	Poster
Turunen, Lotta	Department of Chemistry, NanoScience Center, University of Jyvaskyla, Finnland	DiV_4a
Tyrasa, Swen	Analytik Jena AG, Jena, Germany	Poster
Uecker, Marina	Proteomics Group, Max-Planck-Institute of Experimental Medicine, 37075 Göttingen, Germany	Poster
Uetrecht, Charlotte	Heinrich-Pette-Institut, Hamburg, Deutschland; European XFEL GmbH, Schenefeld, Germany; Heinrich-Pette-Institute, Leibniz Institute for Experimental Virology, Hamburg, Germany	Poster, MiV_3a, Poster, Poster
Uhl, Agnes	Friedrich-Alexander-University Erlangen-Nürnberg, Germany	DiV_1a
Ulbrich, Anne	Universität Rostock, Deutschland	Poster Vortragend
Urlaub, Henning	Max Planck Institute for Biophysical Chemistry, Göttingen, Germany; University Medical Center Göttingen, Germany	DiV_3a, Poster
Uschold, Stephanie	Max Planck Institute for the Structure and Dynamics of Matter CFEL, Hamburg	Poster

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Van Orden, Steve L.	Bruker Daltonics Inc., Billerica, MA, USA	MiV_2a
Van Soest, Remco	SCIEX, USA	Poster
VanOrden, Steve	Bruker Daltonics, Billerica, MA, USA	Poster
Vappiani, Johanna	Cellzome GmbH, Heidelberg	MoN_1a
Vastenhouw, Nadine	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany, Deutschland	MiV_1a
Vaudel, Marc	KG Jebsen Center for Diabetes Research, Department of Clinical Science, University of Bergen, Norway; Center for Medical Genetics and Molecular Medicine, Haukeland University Hospital, Bergen, Norway	DiN_1a
Vendruscolo, Michele	University of Cambridge, United Kingdom	MiV_3a
Venne, A. Saskia	ISAS, Deutschland	MiV_1a
Vennemann, Antje	IBE R&D gGmbH	MoV_2a
Vens-Cappell, Simeon	University of Münster, Insitute for Hygiene, Münster, Germany; Interdisciplinary Center for Clinical Research (IZKF) Münster, Germany	Poster, Poster Vortragend
Verhelst, Steven	ISAS, Deutschland; Department of Cellular and Molecular Medicine, Leuven, Belgium	MiV_1a
Vetere, Alessandro	Max-Planck-Institut für Kohlenforschung, Deutschland	MiV_2a Vortragend
Vialaret, Jerome	Laboratoire de Biochimie et Protéomique Clinique, Institut de Médecine Régénératrice et de Biothérapie, CHU de Montpellier - Hôpital St. Eloi, Montpellier, France	Poster
Vikhnina, Maria	Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry, Germany; Department of Biochemistry, St. Petersburg State University, Russia	Poster Vortragend
Villatoro, José	University of Potsdam, Germany; Bundesanstalt für Materialforschung und -prüfung, Germany; School of Analytical Sciences Adlershof, Germany	Poster Vortragend
Viner, Rosa	Thermo Fisher Scientific, San Jose, CA, USA	Poster
Vissers, Johannes PC	Waters Corporation, Wilmslow, United Kingdom	Poster, Poster
Vitt, Stella	Max Planck Institute of Biophysics, Frankfurt	Poster
Vitz, Jürgen	Friedrich Schiller University Jena, Deutschland	MoN_2a
Vogel, Sarah	Institute of Physiological Chemistry, Faculty of Medicine Carl Gustav Carus, Technical University Dresden, Germany	Poster
Vogt, Thomas	Department of Cell and Metabolic Biology, Leibniz Institute of Plant Biochemistry (Halle/Saale)	DiV_3a
Volmer, Dietrich A.	Saarland University, Saarbrücken, Deutschland	MoN_2a, MoV_4b Vortragend, DiV_2a
von Bergen, Martin	Helmholtz-Centre for Environmental research (UFZ), Department of Molecular Systems Biology, Leipzig, Germany; University of Leipzig, Faculty of Biosciences, Pharmacy and Psychology, Leipzig, Germany; Department for Molecular Systems Biology, Helmholtz Centre for Environmental Research – UFZ, Leipzig, Germany	Poster, Poster
von der Wellen, Jens	Bundeswehr Institute of Pharmacology and Toxicology	Poster Vortragend
von Helden, Gert	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland	MiV_2a, Poster

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Vosse, Christian	Westfälische Wilhelms-Universität Münster, Deutschland	Poster Vortragend
Vu Huu, Khanh	Johann Wolfgang Goethe-Universität, Deutschland	Poster Vortragend
Wachsmuth, Christian J.	University of Regensburg, Institute of Functional Genomics, Regensburg, Deutschland	Poster
Wagner, Anne	Cellzome GmbH, Heidelberg	MoN_1a
Walter, Frederik	Bielefeld University, Bielefeld, Deutschland	Poster
Walter, Ulrich	Center for Thrombosis and Hemostasis, Universitätsklinikum der Johannes Gutenberg-Universität Mainz, Mainz, Germany;	MoN_1a
Walters, David	Fort Collins Science Center, US Geological Survey, Fort Collins, USA	MoV_2b
Wanczek, Karl Peter	Universität Bremen	MiV_2a
Wang, Nan	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster
Wang, Qing	Department of Plant Breeding, Justus Liebig University Giessen, Heinrich-Buff-Ring 26–32, 35392 Giessen, Germany	DiV_2a
Wang, Xiaohang	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster
Wang, Xuxiao	Max-Planck-Institut für Kohlenforschung, Deutschland	MoV_3a Vortragend
Wang, Yuting	Center for Regenerative Therapies, Technical University Dresden, Dresden, Germany; Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany	MoV_1b Vortragend
Warmbrunn, Vera	Friedrich-Alexander-University Erlangen-Nürnberg, Germany	Poster Vortragend
Warzok, Ulrike	Freie Universität Berlin	DiV_4a Vortragend
Watz, Henrik	Pulmonary Research Institute at LungenClinic Großhansdorf, Wöhrendamm 80, 22927 Großhansdorf.; Airway Research Center North, German Center for Lung Research, Wöhrendamm 80, 22927 Großhansdorf, Germany	DiN_3a
Weber, Marcus	Zuse Institute Berlin, Germany	Poster
Weibchen, Gunnar	Waters GmbH, Germany	Poster Vortragend, Poster Vortragend
Weinmann, Wolfgang	Institute of Forensic Medicine, University of Bern; University of Bern, Institute of Forensic Medicine, Forensic Toxicology and Chemistry, Bühlstrasse 20, 3012 Bern, Switzerland; Universtität Bern, Institut für Rechtsmedizin, Forensische Toxikologie und Chemie, Switzerland	Poster, Poster, Poster
Weissflog, Jerrit	Max Planck Institute for Chemical Ecology, Jena, Germany	Poster Vortragend
Weller, Philipp	Hochschule Mannheim, Deutschland	Poster, Poster
Wendt, Juergen	LECO European Application&Technology Center, Berlin, Germany	Poster Vortragend, MiV_2a
Wendt, Karin	Bruker Daltonik GmbH, Deutschland	Poster
Werner, Hauke	Department of Neurogenetics, Max-Planck-Institute of Experimental Medicine, 37075 Göttingen, Germany	Poster
Weske, Sebastian	Georg-August-University Göttingen, Germany	Poster Vortragend
Wessjohann, Ludger A.	Leibniz-Institut für Pflanzenbiochemie, Abteilung Natur- und Wirkstoffchemie, Germany; Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry (Halle/Saale);	DiV_3a, DiV_3a, Poster

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	Leibniz Institute of Plant Biochemistry, Department of Bioorganic Chemistry	
Westphal, Dennis	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig, Germany	Poster Vortragend
Widdig, Anja	Universität Leipzig, Deutschland; Max-Planck-Institut für Evolutionäre Anthropologie, Leipzig, Deutschland; Deutsches Zentrum für integrative Biodiversitätsforschung, Leipzig, Deutschland; German Center for Integrative Biodiversity Research (iDiv), Germany	Poster, Poster
Wiegelmann, Marcel	Institute for Hygiene, Biomedical Mass Spectrometry, University of Münster, Germany	MoV_3b Vortragend, Poster
Wiemann, Martin	IBE R&D gGmbH	MoV_2a
Wildgoose, Jason	Waters Corporation, Wilmslow, United Kingdom	Poster, Poster
Wilharm, Thomas	ASG Analytik Service-Gesellschaft mbH, Neusäss	MiV_2a
Winter, Martin	Institute of Pathology, Christian-Albrechts-Universität, Kiel, Germany	MoV_4b Vortragend
Witt, Matthias	Bruker Daltonik GmbH, Bremen, Germany	MiV_2a, Poster
Wittig, Ilka	Goethe-Universität-Frankfurt	MiV_1a
Wittig, Sabine	Interdisciplinary research center HALOmem, Martin Luther University Halle-Wittenberg, Kurt-Moses-Straße-3, 06120 Halle (Saale).	Poster Vortragend
Wohlfahrt, Sebastian	Helmholtz-Zentrum München,Deutschland	Poster
Wolf, Rainer	Competence Center Analytics, BASF SE, D-67056 Ludwigshafen	Poster Vortragend
Wolters-Eisfeld, Gerrit	University Medical Center Hamburg-Eppendorf, Deutschland	Poster, Poster
Woolerton, Yvonne	Centre for Proteome Research, Institute of Integrative Biology, University of Liverpool, Liverpool, UK	Poster
Wozny, Katharina	Biochemie-Zentrum Heidelberg, Deutschland	MoV_1a Vortragend, Poster
Wrage, Jasmin	GALAB Laboratories GmbH, Deutschland	Poster Vortragend
Wu, Yiman	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster
Wulf, Helena	Universitätsklinikum Schleswig-Holstein, Deutschland	MoV_4b
Wurlitzer, Marcus	University Medical Centre Hamburg-Eppendorf, Institute of Clinical Chemistry, Department for Mass Spectrometric Proteomics, Hamburg Germany	Poster
Wutkowski, Adam	Division of Bioanalytical Chemistry, Research Center Borstel, Parkallee 10, Borstel, Germany	MoV_1b Vortragend
Xu, Xiaoma	Netherlands Forensic Institute, Forensic Chemistry – Chemical Identification Analysis, 2497 GB The Hague, Netherlands	MoN_2a
Xu, Yun	Max-Planck-Institut für Kohlenforschung, Deutschland	Poster Vortragend
Yan, Hao	Heinrich Pette Institute, Leibniz Institute for Experimental Virology, Hamburg, Germany	Poster Vortragend, Poster
Yates, Lisa M.	Princeton University	MoN_1a
Yavor, Mikhail	Institute of Analytical instrumentation, Russian Academy of Sciences, Russia	Poster
Yefremova, Yelena	Proteome Center Rostock, Deutschland	DiV_4a
Young, Phoebe	Goethe Universität Frankfurt, Deutschland	Poster Vortragend
Zahedi, René	Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund, Germany	MoV_4b
Zahedi, René P.	ISAS, Deutschland	MiV_1a Vortragend

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Zahedi, Rene P.	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Deutschland	MoN_1a
Zanni, Thomas	Markes International GmbH, Schleussnerstrasse 42, Frankfurt, Germany	MoN_3a
Zeissig, Sebastian	Center for Regenerative Therapies, Technical University Dresden, Dresden, Germany; Department of Medicine I, University Medical Center Dresden, Technical University Dresden, Dresden, Germany	MoV_1b
Zeller, Martin	Thermo Fisher Scientific, Deutschland	Poster, Poster
Zhao, Shuang	Department of Chemistry, University of Alberta, Edmonton, Canada	Poster
Zheng, Xueyun	Pacific Northwest National Laboratory, USA	DiV_4a
Zimmermann, Ralf	Helmholtz Zentrum Muenchen, Neuherberg; University of Rostock, Rostock	MiV_2a
Zimmermann, Ralf	Joint Mass Spectrometry Centre / Chair of Analytical Chemistry, University of Rostock, 18059 Rostock, Germany; HICE - Helmholtz Virtual of Complex Molecular Systems in Environmental Health – Aerosols and Health, www.hice-vi.eu; Cooperation Group Comprehensive Molecular Analytics, Helmholtz Zentrum München, 85764 Neuherberg, Germany; Universität Rostock, Deutschland; Helmholtz-Zentrum München, Deutschland; 2Joint Mass Spectrometry Centre Helmholtz-Zentrum München, Comprehensive Molecular Analytics (CMA), Neuherberg, Germany	MoN_2a, MoN_3a, Poster, Poster, Poster
Zinn, Nico	Cellzome GmbH, Heidelberg	MoN_1a Vortragend
Zuleger, Nikolaj	MPI of Cell Biology and Genetics, Dresden, Germany	Poster

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Ahrends, Robert	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Germany	A new bridge between targeted and non-targeted LC-MS/MS lipidomics Development of a nanoLC-MS method for global lipidomics PeptideMapper: Efficient and Versatile Amino Acid Sequence and Tag Mapping SIMPLEX reveals myoglobin as a key player in cardiac lipid metabolism
Ambach, Lars	Universtität Bern, Institut für Rechtsmedizin, Forensische Toxikologie und Chemie, Switzerland; Universität Ghent, Department of Bioanalysis, Laboratory of Toxicology, Belgium	Update of an MS/MS Library of NPS for QTRAP® instruments
Angelidou, Georgia	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig; Center for Biotechnology and Biomedicine, Universität Leipzig, Germany	oxLipidomics data integration for systems medicine view on metabolic diseases
Angerer, Verena	Universitätsklinikum Freiburg, Institut für Rechtsmedizin, Forensische Toxikologie, Germany	Update of an MS/MS Library of NPS for QTRAP® instruments
Arlt, Christian	Martin-Luther Universität Halle-Wittenberg, Deutschland; Institute of Pharmacy, Martin Luther University Halle-Wittenberg	An Integrated Mass Spectrometry Based Approach to Probe the Structure of the Full-Length Wild-Type Tetrameric p53 Tumor Suppressor Vortragend An Integrated Workflow for Structural Proteomics Studies based on Cross-linking/Mass Spectrometry with an MS/MS Cleavable Cross-linker
Armeni, Marina	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig; Center for Biotechnology and Biomedicine, Universität Leipzig, Germany	oxLipidomics data integration for systems medicine view on metabolic diseases
Arndt, Birgit	Institute of Food Chemistry, University of Münster, Germany	Algorithms for the annotation of isotopes, fragments and adducts, applied to HPLC-HRMS metabolomics data for the discovery of novel compounds
Arnhold, Jürgen	University of Leipzig, Medical Faculty, Institute of Medical Physics and Biophysics, Härtelstrasse 16- 18, 04107 Leipzig, Germany	Cytochrome c-mediated modification of cardiolipin
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Augsburg, Martina	Medical Systems Biology Medical Faculty, TU Dresden, Dresden, Germany	Absolute quantification of core histones in zebrafish embryos by MS Western
Auth, Thomas	Institut für Organische und Biomolekuare Chemie, Georg-August-Universität Göttingen, Deutschland	An improved approach for calculating dissociation rates of benzylpyridinium ions Vortragend Internal energy of ions produced by electrospray and cryospray ionization

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Bader, Theresa	Helmholtz Zentrum München, Deutschland	Power-function Resolution Filter in Fourier Transform Mass Spectrometry
Baesmann, Carsten	Bruker Daltonik GmbH, Deutschland	Simultaneous quantitation and confirmation of about 500 pesticide residues in food extracts using LC-QTOF accurate mass spectrometry
Bagwan, Navratan	Centro Nacional de investigaciones Cardiovasculares Carlos III (CNIC), Melchor Fernandez Almagro 3, 28029 Madrid, Spain	Software platform to improve the quality control of Lipid mediator quantification
Bahr, Ute	Goethe-Universität-Frankfurt	ArgC-like digestion: complementary or alternative to tryptic digestion? Investigating on-plate digestion of proteins with regard to trypsin activity and oxidation
Bailey, Aaron	Thermo Fisher Scientific, USA	Full Characterization of Antibodies Under Denaturing and Native Conditions on a Hybrid Quadrupole-Orbitrap MS Equipped With a Higher Mass Range
Bajic, Steve	Waters Corporation, United Kingdom	The Aerodynamics of Impactor Spray Ionisation Sources Vortragend
Baker, Erin	Pacific Northwest National Laboratory, USA	Standardised Collision Cross Section Measurements by Single Static Drift Field Ion Mobility Instrument in an Interlaboratory Study
Balcke, Gerd U.	Leibniz-Institut für Pflanzenbiochemie, Stoffwechsel- und Zellbiologie, Germany	Probing plant Maillard reaction by mass spectrometry in model peptide systems
Baldwin, Ian T.	Max Planck Institute for Chemical Ecology, Department for Molecular Ecology, Jena, Germany	Metabolomics to study the “war” between plants and insects - Systemic defense induction and post-ingestive rearrangement of plant toxins in insects.
Bantscheff, Marcus	Cellzome GmbH, Heidelberg	Analysis of drug-induced effects on proteostasis in cell lines and non-dividing primary cells by quantitative mass spectrometry
Barayeu, Uladzimir	University of Leipzig, Medical Faculty, Institute of Medical Physics and Biophysics, Härtelstrasse 16- 18, 04107 Leipzig, Germany	Cytochrome c-mediated modification of cardiolipin Vortragend
Bärenfänger, Melissa	Uni Hamburg, Deutschland	Analysis of human Glycoproteins with different LC-MS/MS and NMR techniques Vortragend
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Bartels, Benjamin	Research Group Mass spectrometry/Proteomics, Max Planck Institute for Chemical Ecology	Mapping metabolites from rough terrain: laser ablation electrospray ionization on non-flat samples Vortragend
Barth, Christof	Justus-Liebig-Universität Gießen, Deutschland	Optimization of the LAMPAS 3 laser mass spectrometer for improved on-line single particle analysis Resolution enhancement by delayed ion extraction in a single-particle aerosol mass spectrometer Vortragend
Baschung, Yannick	Steinbeis Centre Biopolymer Analysis & Biomedical Mass Spectrometry, Rüsselsheim, Germany; Proteome Center, Institute of Immunology, University of Rostock, Rostock, Germany	CHARACTERIZATION OF CARBOHYDRATE BINDING SITES IN GALECTINS BY PROTEOLYTIC AFFINITY - MASS SPECTROMETRY Vortragend

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Baumgarten, Sigrid	Shimadzu Europa GmbH, Deutschland	Analysis of pesticides in food product using SFE-SFC-MSMS
Bayer, Malte	WWU Münster	Pyrylium-based dye and charge tagging in proteomics Vortragend
Baykut, Gökhan	Bruker Daltonik GmbH, Bremen, Germany	2ω-FT-ICR Mass Spectrometry with Quadrupolar Detection MALDI FT-ICR Imaging: Double the Performance or Double the Samples using Quadrupolar Detection
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Beck, Florian	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Deutschland	Temporal quantitative phosphoproteomics of ADP stimulation reveals novel central nodes in platelet activation and inhibition
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Becker, Alexander	Christian-Albrechts-Universität zu Kiel, Deutschland	Improving the sequence coverage in top-down MS/MS of proteins Vortragend
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Begemann, Nora	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	The role of mass spectrometry in the identification of autoantigens as targets in neurological autoimmune diseases Vortragend
Beitz, Toralf	University of Potsdam, Germany	IR-MALDI Ion Mobility Spectrometry: Low and High Field Mobilities of Peptide Ions at Intermediate Pressure
Benninghaus, Thomas	University Medical Center Hamburg-Eppendorf, Deutschland	Application of laser ablation for tissue metabolomics
Berg, Christian	Bruker Daltonics Inc., Billerica, MA, USA	2ω-FT-ICR Mass Spectrometry with Quadrupolar Detection MALDI FT-ICR Imaging: Double the Performance or Double the Samples using Quadrupolar Detection
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Beynon, Robert	Centre for Proteome Research, Institute of Integrative Biology, University of Liverpool, Liverpool, UK	IMS-DIA-MS Characterisation and IMS-MRM QconCAT Quantitation of the Lipidome and Apolipoprotein Complements of Obesity and Diabetes Cohorts
Bhandari, Dhaka ram	Justus Liebig University Giessen, Institute of Inorganic and Analytical Chemistry; Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, Heinrich-Buff-Ring 17, 35392 Giessen, Germany	Differentiating wild and mutant C. elegans using high-resolution atmospheric pressure matrix assisted laser desorption/ionization mass spectrometry imaging Imaging metabolites in wheat stem base-Fusarium graminearum interactions using high-resolution atmospheric pressure scanning microprobe MALDI mass spectrometry imaging (SMALDI-MSI) Vortragend
Bierstedt, Andreas	Bundesanstalt für Materialforschung und -prüfung, Deutschland	Improving the performance of the airborne laser-spark ion source for the detection of volatile organic compounds under ambient conditions Vortragend
Bilova, Tatiana	Leibniz Institute of Plant Biochemistry, Department of Bioorganic Chemistry; Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry (Halle/Saale); Faculty of Chemistry and	Age-related formation of advanced glycation end products (AGEs) in root nodules of common beans (Phaseolus vulgaris) Age-related glycation hotspots in plant proteome Vortragend Probing plant Maillard reaction by mass spectrometry in model peptide systems Simulated microgravity triggers transient enhancement of protein glycation and oxidation in germinating Brassica napus seeds

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	Mineralogy, Universität Leipzig; Department of Plant Physiology and Biochemistry, St. Petersburg State University, Russia; Leibniz-Institut für Pflanzenbiochemie, Abteilung Natur- und Wirkstoffchemie, Germany; Universität Leipzig, Fakultät für Chemie und Mineralogie, Germany	
Birkemeyer, Claudia	Faculty of Chemistry and Mineralogy, Universität Leipzig; Universität Leipzig, Faculty of Chemistry and Mineralogy, Germany; University of Leipzig, Germany	Age-related glycation hotspots in plant proteome Application of LC-MS technique for intra-thallus profiling of polyphenolics in three species of fucoid algae Impact factors on signal response with low temperature plasma ionization for mass spectrometry Methodological aspects of mass spectrometric detection for profiling ambient VOCs with thermodesorption-GCMS Probing plant Maillard reaction by mass spectrometry in model peptide systems The performance of mobile GC-MS for field sampling of body odours from common marmosets (Callithrix jacchus) Vortragend
Bittner, Marian	Freie Universität Berlin, Institute of Pharmacy, Pharmaceutical Biology	UPLC-ESI-QTOF-MS based chemical profiling of Actaea racemosa L. (black cohosh) rhizomes to investigate differences in cultivation, wild harvest, and genotypes Vortragend
Blaum, Bärbel	Interfaculty Institute of Biochemistry, University of Tübingen, Tübingen, Germany	Studying viral capsid glycan interaction with native MS
Böcker, Sebastian	Chair for Bioinformatics, Friedrich Schiller University Jena	Mapping metabolites from rough terrain: laser ablation electrospray ionization on non-flat samples
Bomgarden, Ryan	Thermo Fisher Scientific, Rockford, IL, USA	Optimization of crosslinked peptide analysis on an Orbitrap Fusion Lumos mass spectrometer
Bookmeyer, Christoph H. M.	Institute for Hygiene, University of Münster, Robert-Koch-Str. 41, 48149 Münster, Germany	Single-photon ionization of laser desorbed molecules in a fine-vacuum ion source Vortragend
Boosfeld, Jochen	Bruker Daltonik GmbH, Deutschland	Parts-per-trillion level high-throughput quantitation of glyphosate, aminomethylphosponic acid (AMPA) and glufosinate in water samples by LC-MS/MS Vortragend Simultaneous quantitation and confirmation of about 500 pesticide residues in food extracts using LC-QTOF accurate mass spectrometry Vortragend
Borchard, Nils	Center for International Forestry Research, Indonesia	Historical charcoal additions potentially improve stability of soil organic carbon
Borovinskaya, Olga	TOFWERK, Switzerland	Determination of multi-element composition and mass of single nanoparticles in liquids and air
Borowski, Kathrin	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	The role of mass spectrometry in the identification of autoantigens as targets in neurological autoimmune diseases
Boskamp, Marcel	Institute for Hygiene, University of Münster, Germany	Towards qMALDI-MSI : MS imaging of phospholipids in mouse cerebellum followed by semi-quantitative nano-HPLC-ESI-MS of extracts from laser micro-dissected brain regions Micro-arrays of faux tissue to investigate ion suppression effects in MALDI mass spectrometry of lipids Vortragend
Bowers, Michael T.	University of California, Santa Barbara, USA	The Amyloid Formation Mechanism of Human IAPP: An Infrared Spectroscopy Approach
Brandt, Wolfgang	Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry (Halle/Saale)	Age-related glycation hotspots in plant proteome
Brauch, Dominic	Faculty of Chemistry and Mineralogy, Universität Leipzig; Leibniz Institute of Plant Genetics and Crop Plant Research (Stadt Seeland)	Age-related glycation hotspots in plant proteome

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Brockmann, Eike Ulrich	Institute for Hygiene, Biomedical Mass Spectrometry, University of Münster, Germany	Elucidation of double bond positions in lipids by means of off-line ozonolysis followed by ultraviolet laser desorption ionization mass spectrometry Vortragend
Brogly, Sophie	Hoffmann la Roche AG, Schweiz	Field ionization: an old but still useful method
Brosch, Mario	Department of Medicine I, University Medical Center Dresden, Technical University Dresden, Dresden, Germany	Lipidomics reveals lipid networks correlated with the progression of human colorectal cancer
Brüchert, Stefan	Johann Wolfgang Goethe-Universität, Deutschland	Analyzing macromolecular complexes: subunit interactions of the F1F0 ATP synthase and conformational changes of the heterodimeric ABC transport complex TmrAB
Brügger, Britta	Biochemie-Zentrum Heidelberg, Deutschland	Quantitative Positional Isomer Analysis of Mixed Diacyl-Glycerophospholipids (dGPLs) by Ultra Performance Liquid Chromatography-Electrospray-Tandem Mass Spectrometry (UPLC-ESI-MS/MS) Spotting of Structural Isomer Mixtures of Diacyl-Glycerophospholipids via UPLC-MS/MS
Bruns, Heiko	University Hospital Erlangen, Deutschland	Direct aqueous measurement of 25-hydroxyvitamin D in cellular environments by LC-MS/MS using the novel chemical derivatization reagent MDBP
Bücher, Katharina	Institute for Organic and Macromolecular Chemistry Heinrich-Heine-University Düsseldorf, Düsseldorf Germany	Native mass spectrometry analysis of norovirus - glycan mimetics interaction
Buchholz, Frank	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany, Deutschland; Medical Systems Biology Medical Faculty, TU Dresden, Dresden, Germany	Absolute quantification of core histones in zebrafish embryos by MS Western
Bukowski, Nick	Markes International, Gwaun Elai Medi-Science Campus, Llantrisant, RCT, Wales, United Kingdom	FAST MULTIPLEXING OF IONISATION ENERGY FOR PERFORMANCE IMPROVEMENTS IN GC-TOF MS
Bunse, Christian	Shimadzu Deutschland GmbH, Deutschland	Validierung einer Stabilisotopenverdünnungsanalyse von Folaten in Lebensmitteln und Bestimmung des Folatgehaltes in Naturprodukten Vortragend
Burkhart, Julia M.	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Deutschland	Temporal quantitative phosphoproteomics of ADP stimulation reveals novel central nodes in platelet activation and inhibition
Burmester, Ulrike	Bruker Daltonik GmbH, Deutschland	High resolution trapped ion mobility mass spectrometry analysis of isomeric compounds Vortragend Applying a Proteoform profiling method for neurological disorder biomarker discovery operations Vortragend
Busse, Frederik	Max Planck Institut für Struktur und Dynamik der Materie, Hamburg, Deutschland	Development of Sub-Cellular Mass Spectrometry Imaging by Impulsive IR Laser Ablation Vortragend
Bussmann, Tanja	Research and Development, Beiersdorf AG, Hamburg	Proteomic investigation of skin cell layers by tissue ablation using picosecond infrared laser (PIRL)
Butter, Falk	Institute of Molecular Biology, Deutschland	Proteomic resources for organismal development Vortragend
Buzatto, Adriana	Department of Chemistry, University of Alberta, Edmonton, Canada	Enabling High-Confidence Human Endogenous Metabolite Identification via High-Resolution MS/MS Retention-Time Library
Calleri, Enrica	Department of Drug Sciences, University of Pavia, Pavia, Italy	Innovative analytical methodologies for the development of new antitubercular agents
Campidelli, Stéphane	LICSEN, NIMBE, CEA, CNRS, Université Paris-Saclay, France	Formate attachment to ZnPorphyrin- and ZnPhthalocyanine-Oligomers: Binding, Fragmentation, Affinity
Cannistraci, Carlo V.	Biomedical Cybernetics Group, Biotechnology Center, Technical University Dresden, Dresden, Germany	Lipidomics reveals lipid networks correlated with the progression of human colorectal cancer
Cassidy, Liam Arron	AG Systematische Proteomforschung &	Quantitative proteomics for the analysis of molecular changes in lung adenocarcinoma cells in response to Vitamin D3

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	Bioanalytik, Institut für Experimentelle Medizin, Christian-Albrechts-Universität, Kiel	Combining 2D-LC-MS and Gelfree-LC-MS enhances both proteome coverage and the identification of short open reading frame encoded peptides Vortragend
Castro-Perez, Jose	Waters Corporation, Milford, MA	IMS-DIA-MS Characterisation and IMS-MRM QconCAT Quantitation of the Lipidome and Apolipoprotein Complements of Obesity and Diabetes Cohorts
Causon, Tim	BOKU Wien, Österreich	Standardised Collision Cross Section Measurements by Single Static Drift Field Ion Mobility Instrument in an Interlaboratory Study Vortragend
Chait, Brian T.	The Rockefeller University, New York, USA	Integrative Methods for Elucidating the Structure & Function of Cellular Machines Vortragend
Chantseva, Veronika	Department of Plant Physiology and Biochemistry, St. Petersburg State University	Simulated microgravity triggers transient enhancement of protein glycation and oxidation in germinating Brassica napus seeds Vortragend
Chen, Yu-Ju	Academia Sinica, School of Chemistry, Taipei, Taiwan	Increased confidence for the identification of N-linked glycopeptides using an optimised collision energy workflow Increased confidence for the identification of N-linked glycopeptides using an optimised collision energy workflow
Chernev, Aleksandar	Max Planck Institute for Biophysical Chemistry, Göttingen, Germany	Analysis of UV-induced DNA–protein cross-links in a chromatin model Analysis of 1,2,3,4-diepoxybutane induced DNA-histone cross-links by mass spectrometry
Chervet, Jean-Pierre	ANTEC, Leyden	In situ monitoring of lipid oxidation using electrochemistry-mass spectrometry coupling
Ciucci, Sara	Biomedical Cybernetics Group, Biotechnology Center, Technical University Dresden, Dresden, Germany; Lipotype GmbH, Dresden, Germany	Lipidomics reveals lipid networks correlated with the progression of human colorectal cancer
Claassen, Christin	GALAB Laboratories GmbH, Deutschland	Discrimination of apple and potato cultivars by non-targeted metabolomic fingerprinting via UPLC-IMS-QToF analysis
Claude, Emmanuelle	Waters Corporation, United Kingdom	Getting DESI Imaging up to speed for clinical applications
Clemen, Martin	Christian-Albrechts-Universität zu Kiel, Institut für Physikalische Chemie, Max-Eyth-Str. 1, 24118 Kiel, Deutschland	Energetische und kinetische Betrachtung der Fragmentierung von Azofarbstoffen mit Diethylamino Gruppe Vortragend
Coliva, Giulia	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig; Center for Biotechnology and Biomedicine, Universität Leipzig, Germany	In situ monitoring of lipid oxidation using electrochemistry-mass spectrometry coupling Vortragend oxLipidomics data integration for systems medicine view on metabolic diseases
Colombo, Simone	Mass Spectrometry Centre, Department of Chemistry & QOPNA, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal	In situ monitoring of lipid oxidation using electrochemistry-mass spectrometry coupling
Coman, Cristina	Leibniz-Institut für Analytische Wissenschaften – ISAS e.V., Germany	SIMPLEX reveals myoglobin as a key player in cardiac lipid metabolism Vortragend
Conway, Debra	Analytik Jena AG, Jena, Germany	Ultra High Throughput Drug Discovery Screening by MALDI-TOF Mass Spectrometry
Cornett, Shannon	Bruker Daltonics, Billerica, MA, USA	MALDI FT-ICR Imaging: Double the Performance or Double the Samples using Quadrupolar Detection
Cramer, Benedikt	Institute of Food Chemistry, University of Münster, Germany	Localization of Ergot Alkaloids in Sclerotia of Claviceps purpurea by MALDI-MS Imaging
Crawford, Elizabeth	Saarland University, Saarbrücken, Deutschland	Rapid fingerprinting of lignin renewable energy sources by ambient ionization high-resolution mass spectrometry and simplified data mining Vortragend
Crecelius, Anna C.	Friedrich Schiller University Jena, Deutschland	Effect of ecosystem type and fire on chemistry of WEOM as measured by LDI-TOF-MS and NMR Vortragend

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Creutznacher, Robert	Institute of Chemistry, University of Lübeck, Lübeck, Germany	Native mass spectrometry analysis of norovirus - glycan mimetics interaction
Crone, Barbara	Institut für Anorganische und Analytische Chemie, Universität Münster, Deutschland	Investigating the zinc distribution in the mayfly N. triangulifer using elemental bioimaging by LA-ICP-MS Vortragend
Czech, Hendryk	Universität Rostock, Deutschland	Direct resonance-enhanced multi-photon ionisation (REMPI) of complex liquid samples under vacuum conditions Vortragend
Damoc, Eugen	Thermo Fisher Scientific, Deutschland	Evaluation of Optimal Conditions for Antibody Subunit Analysis on a Quadrupole-Orbitrap Mass Spectrometer Full Characterization of Antibodies Under Denaturing and Native Conditions on a Hybrid Quadrupole-Orbitrap MS Equipped With a Higher Mass Range
Danne-Rasche, Niklas	Leibniz Institut für Analytische Wissenschaften ISAS e.V.	Development of a nanoLC-MS method for global lipidomics Vortragend
Danquah, Bright D.	Proteome Center Rostock, Deutschland	Intact Transition Epitope Mapping - A mass spectrometric method for accurate, facile, and rapid identification of specific antibody-peptide reactivities
Danz, Norbert	Fraunhofer Institute for Applied Optics and Precision Engineering IOF	Mapping metabolites from rough terrain: laser ablation electrospray ionization on non-flat samples
Darland, Ed	Agilent Technologies, Santa Clara, USA	Standardised Collision Cross Section Measurements by Single Static Drift Field Ion Mobility Instrument in an Interlaboratory Study
De Angelis, Francesco	Dipart. di Sci. Fisiche e Chimiche, Università degli Studi dell'Aquila, Via Vetoio, Coppito, 67100 L'Aquila, Italy	COPPER-CATALYSED CLICK REACTION PERFORMED IN THE GAS PHASE: A COMBINED MASS SPECTROMETRIC AND DFT MECHANISTIC STUDY
de Bruyn, René	Netherlands Forensic Institute, Forensic Chemistry – Chemical Identification Analysis, 2497 GB The Hague, Netherlands	Development and implementation of new analytical methods and databases for the detection of additives in fuels and fire debris.
Decker, Petra	Bruker Daltonik GmbH, Deutschland	Simultaneous quantitation and confirmation of about 500 pesticide residues in food extracts using LC-QTOF accurate mass spectrometry
Dedishov, Ruslan	Markes International GmbH, Schleussnerstrasse 42, Frankfurt, Germany	FAST MULTIPLEXING OF IONISATION ENERGY FOR PERFORMANCE IMPROVEMENTS IN GC-TOF MS
Dell'Aica, Margherita	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Deutschland	Temporal quantitative phosphoproteomics of ADP stimulation reveals novel central nodes in platelet activation and inhibition
Denno, Yvonne	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	The role of mass spectrometry in the identification of autoantigens as targets in neurological autoimmune diseases
Desbenoit, Nicholas	Universität Bayreuth, Deutschland	Multimodal imaging combining mass spectrometry and vibrational spectroscopy using a single tissue section and an integrated data processing workflow
Desbenoit, Nicolas	Chair of Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth, Germany	Overview of imzML-based software tools for MS imaging imzML - Current status and future perspectives of the open standard for mass spectrometry imaging data
Dettmer, Katja	University of Regensburg, Institute of Functional Genomics, Regensburg, Deutschland	A step forward in GC-HRAM-MS based metabolomics - A novel atmospheric pressure GC-APCI Source increases quantitative and qualitative performance
Diarra, David	Oil-Wärme-Institut GmbH, Herzogenrath, Deutschland	Thermogravimetry coupled to Ultrafast Gas Chromatography Singlephoton-Ionisation Time-of-Flight-Mass-Spectrometry (TG-SPI-TOF-MS) for Evolved-Gas-Analysis of Fuels regarding to the Deposit Formation Potential
Dickel, Timo	II physikalisches Insitut, Justus-Liebig-Universität Gießen, Deutschland; GSI Darmstadt, Deutschland	Tandem Mass Spectrometry with a (Ultra-)High Resolving Time-of-Flight Mass Spectrometer
DiConza, Giusy	Laboratory of Molecular Oncology and Angiogenesis, Vesalius Research Center, Leuven, Belgium	Excellent sensitivity through excellent recovery – ERLIC for absolute quantification of low abundant protein phosphorylation events in cancer patient tissue

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Didio, Anna	Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry; Department of Biochemistry, St. Petersburg State University	Simulated microgravity triggers transient enhancement of protein glycation and oxidation in germinating Brassica napus seeds
Dietrich, Dörthe	Westfälische Wilhelms-Universität Münster	Imaging of Cerium Oxide Nanoparticles and Phospholipids in Rat Lung Tissue by Means of LA-ICP-MS and MALDI-MS Vortragend
Ding, Xuelu	Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen	Reactive low temperature plasma (LTP) mass spectrometry of neurosteroids Vortragend
Dinse, Martin	PerkinElmer LAS (Germany) GmbH, Deutschland	Rapid On Site Analysis of BTX with Portable GC/MS Vortragend
Dirk, Tänzler	Martin-Luther-University Halle-Wittenberg, Institute of Pharmacy, Department of Pharmaceutical Chemistry and Bioanalytics, Germany	Structural Insights into Retinal Guanylyl Cyclase/GCAP-2 Interaction by Cross-linking and Mass Spectrometry
Disko, Ulrich	Forschungszentrum Jülich, Deutschland	Historical charcoal additions potentially improve stability of soil organic carbon
Dojahn, Joerg	SCIEX, Deutschland	Accelerating Data Independent Acquisition with Microflow Chromatography Vortragend
Domingues, M. Rosario	Mass Spectrometry Centre, Department of Chemistry & QOPNA, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal	In situ monitoring of lipid oxidation using electrochemistry-mass spectrometry coupling
Domingues, Pedro	Mass Spectrometry Centre, Department of Chemistry & QOPNA, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal	In situ monitoring of lipid oxidation using electrochemistry-mass spectrometry coupling
Dopstadt, Julian	Institute of Food Chemistry, University of Münster, Germany	Localization of Ergot Alkaloids in Sclerotia of Claviceps purpurea by MALDI-MS Imaging
Dral, Pavlo O.	Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany	Reactivity and stability check of even vs. odd electron (quasi)-molecular ions derived from triangulenium type derivatives
Drechsel, David	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany, Deutschland; Present address: IMP Research Institute of Molecular Pathology, 1030 Vienna, Austria	Absolute quantification of core histones in zebrafish embryos by MS Western
Dreger, Mathias	caprotec bioanalytics GmbH	Metal labelling of tri-functional Capture Compounds (CCs) to detect protein targets of small molecules
Dreisewerd, Klaus	University of Münster, Institute of Hygiene, Biomedical Mass Spectrometry, Germany; Interdisciplinary Center for Clinical Research (IZKF) Münster, Germany; Institute for Hygiene, University of Münster, Germany; Institute for Hygiene, University of Münster, Robert-Koch-Str. 41, 48149 Münster, Germany	Colorful MALDI: Effect of the Laser Excitation Wavelength on the Analytical Sensitivity in Standard MALDI-MS and Imaging Experiments Localization of Ergot Alkaloids in Sclerotia of Claviceps purpurea by MALDI-MS Imaging Micro-arrays of faux tissue to investigate ion suppression effects in MALDI mass spectrometry of lipids Single-photon ionization of laser desorbed molecules in a fine-vacuum ion source The internal energy in a MALDI plume probed with thermometer molecules: Effects of laser excitation wavelength and laser fluence Towards qMALDI-MSI : MS imaging of phospholipids in mouse cerebellum followed by semi-quantitative nano-HPLC-ESI-MS of extracts from laser micro-dissected brain regions CoolMALDI: Combination of IR-ablation and UV-postionization of snap-frozen tissue sections for sensitive imaging of lipids and metabolites Elucidation of double bond positions in lipids by means of off-line ozonolysis followed by ultraviolet laser desorption ionization mass spectrometry New insights into the MALDI mechanisms: Postionization and

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		photoacoustic experiments reveal laser spot size-dependent transitions between desorption and ablation regimes
Drewello, Thomas	Friedrich-Alexander-University Erlangen-Nürnberg, Deutschland	Aggregation of a crown-ether decorated zinc-phthalocyanine by collision-induced desolvation providing insight into the electrospray mechanism Formate attachment to ZnPorphyrin- and ZnPhthalocyanine-Oligomers: Binding, Fragmentation, Affinity Formation and dissociation behavior of multiply charged salt-like cluster ions (sodium formate) Formation and structure elucidation of $[M_2$ and $Ag]^+$ ions with M = [6]helicene, [7]helicene and coronene Reactivity and stability check of even vs. odd electron (quasi)-molecular ions derived from triangulenium type derivatives
Dreyer, Benjamin	University Medical Center Hamburg-Eppendorf, Deutschland	Comparison of label free quantification methods for proteomics Mass spectrometric characterization of aberrant O-glycosylation in COSMC deficient mouse pancreas tissue Vortragend
Dülcks, Thomas	Universität Bremen, Deutschland	Separation and identification of muscarine isomers Vortragend
Dunn, Adrian	Departments of Platform Technology & Science, GlaxoSmithKline, Stevenage, UK	Ultra High Throughput Drug Discovery Screening by MALDI-TOF Mass Spectrometry
Dürr, Maximilian	Friedrich-Alexander-University Erlangen-Nürnberg, Deutschland	Aggregation of a crown-ether decorated zinc-phthalocyanine by collision-induced desolvation providing insight into the electrospray mechanism
Duschl, Wolfgang J.	Christian-Albrechts-Universität zu Kiel, Deutschland	Where are ye all? – On the (serious) search for extraterrestrial life Vortragend
Dwayne Miller, R. J.	Max Planck Institute for the Structure and Dynamics of Matter CFEL, Hamburg	Proteomic investigation of skin cell layers by tissue ablation using picosecond infrared laser (PIRL)
Easterling, Michael L.	Bruker Daltonics, Billerica, MA, USA	MALDI FT-ICR Imaging: Double the Performance or Double the Samples using Quadrupolar Detection 2ω-FT-ICR Mass Spectrometry with Quadrupolar Detection
Eble, Johannes	Institut für Physiologische Chemie und Pathobiochemistry, Universität Münster, Deutschland	Identification of an unusual N-glycan detected in a tryptic glycopeptide derived from intergrin α7 expressed in Drosophila S2 cells
Eckelmann, Paula	Federal Criminal Police Office, Forensic Institute, 65193 Wiesbaden, Germany; Justus-Liebig-University Giessen, Institute of Food Chemistry and Food Biotechnology, 35392 Giessen, Germany	Development and implementation of new analytical methods and databases for the detection of additives in fuels and fire debris.
Eckey, Kevin	Universität Münster, Deutschland	Investigations on the photolysis of sulfamethoxazole Vortragend
Edler, Stefan	LAS Perkinelmer GmbH, Deutschland	Rapid Screening of Methylamphetamine in Hair of Drug Addicts using DSA-TOF Vortragend
Eggers, Lars Florian	Research Center Borstel, Division of Bioanalytical Chemistry, Parkallee 1-40, D-23845 Borstel, Germany.	Lipidomes of human lung tissues show distinct lipid metabolic alterations for lung cancer and pulmonary emphysema Vortragend
Eggert, Dennis	Heinrich Pette Institute, Leibniz Institute for Experimental Virology, Hamburg	Proteomic investigation of skin cell layers by tissue ablation using picosecond infrared laser (PIRL)
Eiersbrock, Fabian	Institute for Hygiene, Uni Münster, Germany	Micro-arrays of faux tissue to investigate ion suppression effects in MALDI mass spectrometry of lipids Towards qMALDI-MSI : MS imaging of phospholipids in mouse cerebellum followed by semi-quantitative nano-HPLC-ESI-MS of extracts from laser micro-dissected brain regions Vortragend
Einspanier, Almuth	Universität Leipzig, Deutschland	The performance of mobile GC-MS for field sampling of body odours from common marmosets (Callithrix jacchus)
El-Khatib, Ahmed	Humboldt-Universität zu Berlin, Institut für Chemie, Deutschland	A new internal standard approach for laser ablation ICP-MS of polyacrylamide gels Mass Spectrometry Imaging as Tool for the Analysis of MRI Contrast Agents in Biological Tissues
Enders, Claudia	Merck KGaA, Frankfurter Str. 250, 64293 Darmstadt, Germany	Analysis of Liquid Crystal Display Sealants using Spatially Resolved Mass Spectrometric Methods

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Engeser, Marianne	Universität Bonn, Deutschland	ETD experiments on self-assembled asymmetric supramolecular squares One-electron reduction of isolated metallo-supramolecular aggregates Vortragend
Ermler, Ulrich	Max Planck Institute of Biophysics, Frankfurt	From Salty to Salt-free: Monitoring the Salt-dependent Dissoziation of the Membrane Protein Complex GCD in a Single Experiment
Esch, Patrick	Institute of Inorganic and Analytical Chemistry, Justus-Liebig-University, Giessen, Germany	Charge Switching of Phospholipids using Paternó-Büchi Reactions Vortragend
Escher, Beate	Helmholtz-Centre for Environmental research (UFZ), Department of Cell Toxicology, Leipzig, Germany	Phthalate metabolites MEHP and MEOHP but not the phthalate DEHP itself bind and activate the PPARγ
Esfeld, Sonja	University Hospital Essen, Medical Faculty, West German Heart and Vascular Center, Department of Cardiology and Department of Angiology, Germany	SIMPLEX reveals myoglobin as a key player in cardiac lipid metabolism
Etienne, Chris	Thermo Fisher Scientific, Rockford, IL, USA	Optimization of crosslinked peptide analysis on an Orbitrap Fusion Lumos mass spectrometer
Faelth-Savitski, Maria	Cellzome GmbH, Heidelberg	Analysis of drug-induced effects on proteostasis in cell lines and non-dividing primary cells by quantitative mass spectrometry
Fagbadebo, Funmilayo	Leibniz-Institut für Pflanzenbiochemie, Abteilung Natur- und Wirkstoffchemie, Germany	Probing plant Maillard reaction by mass spectrometry in model peptide systems
Farmani, Zahra	Bio-film Center Universität Duisburg-Essen; Max-Planck-Institut für Kohlenforschung, Germany	Metabolite analysis of the phenanthrene degrading, sulfate reducing bacterial enrichment culture (TRIP) using GC-MS Vortragend
Fatangare, Amol	Chair of Bioanalytical Sciences and Food Analysis, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth, Germany	imzML - Current status and future perspectives of the open standard for mass spectrometry imaging data Overview of imzML-based software tools for MS imaging Vortragend
Fazel, Ramin	The University of Tehran, Iran; Universitätsklinikum Hamburg-Eppendorf, Germany	Mass spectrometry evaluation of the Etanercept physicochemical properties Vortragend
Fedorova, Maria	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig, Germany; Center for Biotechnology and Biomedicine, Universität Leipzig, Germany	Identification of oxidative biomarkers in synovial fluid of patients suffering from rheumatoid arthritis In situ monitoring of lipid oxidation using electrochemistry-mass spectrometry coupling oxLipidomics data integration for systems medicine view on metabolic diseases Vortragend
Fiedler, Dorothea	Leibniz-Institut für molekulare Pharmakologie (FMP), Deutschland; Humboldt-Universität zu Berlin; Princeton University	Neutral loss-triggered EThcD mass spectrometry identifies protein pyrophosphorylation in vivo
Fielitz, Davor	Shimadzu Deutschland GmbH, Deutschland	Analysis of pesticides in food product using SFE-SFC-MSMS Vortragend
Firl, Nina	Shimadzu Deutschland GmbH, Deutschland	Validierung einer Stabilisotopenverdünnungsanalyse von Folaten in Lebensmitteln und Bestimmung des Folatgehaltes in Naturprodukten
Fischer, Michael	Helmholtz-Zentrum München,Deutschland	Thermogravimetry coupled to Ultrafast Gas Chromatography Singlephoton-Ionisation Time-of-Flight-Mass-Spectrometry (TG-SPI-TOF-MS) for Evolved-Gas-Analysis of Fuels regarding to the Deposit Formation Potential
Fischer, Moritz	Universität zu Köln, Deutschland	Synthesis of Isotope-Labeled Derivatives of the MS/MS-Cleavable Urea-Cross-Linker: Synthesis and Evaluation of Reactivity for Effective Protein Structure Analysis Vortragend
Fischle, Wolfgang	Max Planck Institute for Biophysical Chemistry, Göttingen, Germany; KAUST, Saudi Arabia	Analysis of UV-induced DNA–protein cross-links in a chromatin model
Fjeldsted, John	Agilent Technologies, Santa Clara, USA	Standardised Collision Cross Section Measurements by Single Static Drift Field Ion Mobility Instrument in an Interlaboratory Study

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Flemmig, Jörg	University of Leipzig, Medical Faculty, Institute of Medical Physics and Biophysics, Härtelstrasse 16- 18, 04107 Leipzig, Germany	Cytochrome c-mediated modification of cardiolipin
Folberth, Julica	University of Lübeck, Germany	LC/MS²-standards library using high-resolution accurate mass (HRAM) platform for metabolomics research Vortragend
Franken, Holger	Cellzome GmbH, Heidelberg	Analysis of drug-induced effects on proteostasis in cell lines and non-dividing primary cells by quantitative mass spectrometry
Franz, Florian	Universitätsklinikum Freiburg, Institut für Rechtsmedizin, Forensische Toxikologie, Germany	Update of an MS/MS Library of NPS for QTRAP® instruments
Franzke, Joachim	Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V.	Analyse des Peroxid-basierten Sprengstoffs TATP und strukturell verwandter Verbindungen mittels dielektrisch behinderter Entladungsionisations-Massenspektrometrie (DBDI-MS)
Fraune, Sebastian	Zoologisches Institut, Uni Kiel	Identification and characterization of N-acyl homoserine lactones by mass spectrometry
Frensemeier, Lisa	Universität Münster, Deutschland	Electrochemical conversion of Pt(IV) prodrugs to Pt(II) cytostatics investigated by means of liquid chromatography and mass spectrometry Vortragend
Freund, Christian	Institut für Chemie und Biochemie, Freie Universität Berlin, Deutschland	Analysis of serine-phosphorylation dependent protein-protein interactions of the T cell adaptor protein ADAP
Friedrich, Jochen	Bruker Daltonik GmbH, Bremen, Germany	2ω-FT-ICR Mass Spectrometry with Quadrupolar Detection Vortragend MALDI FT-ICR Imaging: Double the Performance or Double the Samples using Quadrupolar Detection
Frolov, Andrej	Leibniz-Institut für Pflanzenbiochemie, Abteilung Natur- und Wirkstoffchemie, Germany; Universität Leipzig, Fakultät für Chemie und Mineralogie, Germany	Probing plant Maillard reaction by mass spectrometry in model peptide systems Vortragend
Frolov, Andrej	Leibniz Institute of Plant Biochemistry, Department of Bioorganic Chemistry; Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry (Halle/Saale); Faculty of Chemistry and Mineralogy, Universität Leipzig	Age-related formation of advanced glycation end products (AGEs) in root nodules of common beans (Phaseolus vulgaris) Age-related glycation hotspots in plant proteome Profiles of glycated amino acid adducts in the protein hydrolyzates of pea (Pisum sativum) seeds subjected to accelerated ageing Simulated microgravity triggers transient enhancement of protein glycation and oxidation in germinating Brassica napus seeds
Fuchs, M.	2Joint Mass Spectrometry Centre Helmholtz-Zentrum München, Comprehensive Molecular Analytics (CMA), Neuherberg, Germany	Multiple analysis of individual airborne aerosol particles by laser mass spectrometry: Detection of polyaromatic hydrocarbons from the particle-surface and particle-core
Fuchs, Sabine	Klinik für Unfallchirurgie und Traumatologie, Experimentelle Unfallchirurgie, UKSH, Kiel	Quantitative proteomics for the analysis of molecular changes in lung adenocarcinoma cells in response to Vitamin D3
Fuchser, Jens	Bruker Daltonik GmbH, Bremen, Germany	2ω-FT-ICR Mass Spectrometry with Quadrupolar Detection Ultra High Throughput Drug Discovery Screening by MALDI-TOF Mass Spectrometry
Fuetterer, Arne	Bruker Daltonik GmbH, Germany	Ultra High Throughput Drug Discovery Screening by MALDI-TOF Mass Spectrometry
Fufezan, Christian	Institute for Biology and Biotechnology of Plants, University Münster, Münster, Germany;	Temporal quantitative phosphoproteomics of ADP stimulation reveals novel central nodes in platelet activation and inhibition
Fuh, Marceline Manka	University Medical Centre Hamburg-Eppendorf, Institute of Clinical Chemistry, Department for Mass Spectrometric Proteomics, Hamburg Germany	Lipidomics of Pig Brain Using the PIRL-DIVE Homogenisation Technique Vortragend
Furrer, Julien	Department of Chemistry and Biochemistry, University of Bern	N-Acetyltaurine as a novel urinary ethanol marker in a drinking study

Autor(en)	Organisation(en)	Titel des Beitrags
Gabelica, Valérie	Inserm, CNRS, Université de Bordeaux, Laboratoire "Acides Nucléiques, Régulations Naturellee et Artificielle" (ARNA, U1212, UMR5320), IECB, Pessac, France	Nucleic acids biophysics: insight from (and into) mass spectrometry Vortragend
Gabelle, Audrey	Laboratoire de Biochimie et Protéomique Clinique, Institut de Médecine Régénératrice et de Biothérapie, CHU de Montpellier - Hôpital St. Eloi, Montpellier, France; Centre Mémoire Ressources Recherche, CHU Montpellier, hôpital Gui de Chauliac, Montpellier, France	Applying a Proteoform profiling method for neurological disorder biomarker discovery operations
Gade, Stephan	Cellzome GmbH, Heidelberg	Analysis of drug-induced effects on proteostasis in cell lines and non-dividing primary cells by quantitative mass spectrometry
Gallaspy, Alan	PerkinElmer LAS (Germany) GmbH, Deutschland	Rapid On Site Analysis of BTX with Portable GC/MS
Galyamova, Aigerim	Pennsylvania State University, USA	Impact factors on signal response with low temperature plasma ionization for mass spectrometry
Gambaryan, Stepan	Sechenov Institute of Evolutionary Physiology and Biochemistry, Russian Academy of Sciences, Saint Petersburg, Russia;	Temporal quantitative phosphoproteomics of ADP stimulation reveals novel central nodes in platelet activation and inhibition
Gaquerel, Emmanuel	Centre for Organismal Studies Heidelberg, University of Heidelberg, Germany	Metabolomics to study the “war” between plants and insects - Systemic defense induction and post-ingestive rearrangement of plant toxins in insects.
Garbeva, Paolina	Department of Microbial Ecology, Netherlands Institute of Ecology, Wageningen, The Netherlands	Application of high-throughput MS screening to disentangle the bacterial metabolome
Garcia Alai, Maria Marta	European Molecular Biology Laboratory (EMBL), Hamburg, Germany	Structural characterization of protein-lipid complexes involved in clathrin-mediated endocytosis
Geiger, Jörg	Interdisciplinary Bank of Biomaterials and Data, Würzburg, Germany;	Temporal quantitative phosphoproteomics of ADP stimulation reveals novel central nodes in platelet activation and inhibition
Geissel, Hans	II physikalisches Insitut, Justus-Liebig-Universität Gießen, Deutschland; GSI Darmstadt, Deutschland	Tandem Mass Spectrometry with a (Ultra-)High Resolving Time-of-Flight Mass Spectrometer
Gentzel, Marc	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany, Deutschland; Present address: Center for Molecular and Cellular Bioengineering, TU Dresden, 01307 Germany	Absolute quantification of core histones in zebrafish embryos by MS Western
Gerbig, Stefanie	Justus Liebig University, Gießen, Deutschland	Rapid fingerprinting of lignin renewable energy sources by ambient ionization high-resolution mass spectrometry and simplified data mining Real-time food authentication with a miniature mass spectrometer Vortragend
Gerbig, Stefanie	Justus-Liebig-Universität Gießen, Institut für Anorganische und Analytische Chemie	AP-SMALDI MSI of metabolites and lipids in Schistosoma mansoni parasites
Gerhardt, Natalie	Hochschule Mannheim, Deutschland	Quality assessment of olive oil based on volatile compound fingerprinting using HRGC-IMS analysis Vortragend
Gethings, Lee	Waters Corporation, Wilmslow, United Kingdom	Lipidomics Quantitation Using a Novel Scanning Quadrupole DIA Method Quantitation of Proteomics Samples Using a Novel Scanning Quadrupole DIA Method
Gethings, Lee A	Waters, Wilmslow, UK	Increased confidence for the identification of N-linked glycopeptides using an optimised collision energy workflow IMS-DIA-MS Characterisation and IMS-MRM QconCAT Quantitation

Autor(en)	Organisation(en)	Titel des Beitrags
		of the Lipidome and Apolipoprotein Complements of Obesity and Diabetes Cohorts
Gewinner, Sandy	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland	Glycan Fingerprinting using Cold-Ion Infrared Spectroscopy
Gieras, Anna	European Molecular Biology Laboratory (EMBL), Hamburg, Germany	Structural characterization of protein-lipid complexes involved in clathrin-mediated endocytosis
Glocker, Michael	Proteome Center, Institute of Immunology, University of Rostock, Rostock, Germany	Innovative analytical methodologies for the development of new antitubercular agents
Glocker, Michael O.	Proteome Center Rostock, Deutschland	Intact Transition Epitope Mapping - A mass spectrometric method for accurate, facile, and rapid identification of specific antibody-peptide reactivities Vortragend
Göbel, Michael	Goethe-Universität Frankfurt, Deutschland	Steps towards a more native analysis of Aß42 using LILBID mass spectrometry
Goldmann, Torsten	Pathology of the University Hospital of Lübeck and the Research Center Borstel, Clinical and Experimental Pathology, 23538 Lübeck and 23845 Borstel, Germany.; Airway Research Center North, German Center for Lung Research, Wöhrendamm 80, 22927 Großhansdorf, Germany	Lipidomes of human lung tissues show distinct lipid metabolic alterations for lung cancer and pulmonary emphysema
Golghalyani, Vahid	Goethe-Universität-Frankfurt	ArgC-like digestion: complementary or alternative to tryptic digestion? Vortragend A versatile method to extract, modify, enrich and digest proteomic samples directly from cell lysates
Gonzalez Florez, Ana Isabel	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland	Glycan Fingerprinting using Cold-Ion Infrared Spectroscopy
Goseli, Christoph	Bruker BioSpin, Fällanden, Switzerland	MALDI FT-ICR Imaging: Double the Performance or Double the Samples using Quadrupolar Detection
Gosteli, Christoph	Bruker BioSpin AG, Fällanden, Switzerland	2ω-FT-ICR Mass Spectrometry with Quadrupolar Detection
Göth, Melanie	Freie Universität Berlin, Deutschland; Fritz-Haber-Institut Berlin, Deutschland	Following the Unfolding and Dissociation of Calmodulin/Munc13 Complexes by Ion Mobility-Mass Spectrometry Vortragend
Gottfried, Sebastian	Waters Corporation, United Kingdom	Getting DESI Imaging up to speed for clinical applications Vortragend
Gottwald, Sven	Department of Plant Breeding, Justus Liebig University Giessen, Heinrich-Buff-Ring 26–32, 35392 Giessen, Germany	Imaging metabolites in wheat stem base-Fusarium graminearum interactions using high-resolution atmospheric pressure scanning microprobe MALDI mass spectrometry imaging (SMALDI-MSI)
Götze, Michael	Institute of Biochemistry, Martin Luther University Halle-Wittenberg	An Integrated Workflow for Structural Proteomics Studies based on Cross-linking/Mass Spectrometry with an MS/MS Cleavable Cross-linker
Grafinger, Katharina	Universtität Bern, Institut für Rechtsmedizin, Forensische Toxikologie und Chemie, Switzerland	Update of an MS/MS Library of NPS for QTRAP® instruments Vortragend
Grevelding, Christoph	Justus-Liebig-Universität Gießen, Institut für Parasitologie	AP-SMALDI MSI of metabolites and lipids in Schistosoma mansoni parasites
Grishina, Tatiana	Universität St. Petersburg, Lehrstuhl Biochemie, Russia; Department of Biochemistry, St. Petersburg State University	Probing plant Maillard reaction by mass spectrometry in model peptide systems Simulated microgravity triggers transient enhancement of protein glycation and oxidation in germinating Brassica napus seeds
Groessl, Michael	Tofwerk, Uttigenstrasse 22, CH-3600 Thun, Switzerland	Differentiation and relative quantification of chondroitin sulfate isomers by ion mobility spectrometry-mass spectrometry and pulsed-field gradient NMR Separation of isomeric cannabinoids by high-resolution ion mobility-MS for the differentiation of legal and illegal marijuana

Autor(en)	Organisation(en)	Titel des Beitrags
Gröger, Thomas	Helmholtz Zentrum Muenchen, Neuherberg	The Usage of Direct Inlet Probe in combination with High Resolution Mass Spectrometry for the Characterization of Heavy Petroleum Products
Grosche, Julius	Institut für Physiologische Chemie und Pathobiochemistry, Universität Münster, Deutschland	Identification of an unusual N-glycan detected in a tryptic glycopeptide derived from intergrin α7 expressed in Drosophila S2 cells
Gross, Jürgen	Universität Heidelberg, Deutschland	Evaluierung basischer Polypropylenglycole als Standards zur internen Kalibrierung für exakte Massen in der positiv-Ionen MALDI-TOF-MS Vortragend
Grotemeyer, Jürgen	Christian-Albrechts-Universität zu Kiel, Institut für Physikalische Chemie, Max-Eyth-Str. 1, 24118 Kiel, Deutschland; Universität Kiel, Deutschland	Energetische und kinetische Betrachtung der Fragmentierung von Azofarbstoffen mit Diethylamino Gruppe REMPI- und MATI-Spektroskopie an den Methylpyridinen REMPI-Spektroskopie von nicht-kovalenten Anisol-Clustern Untersuchung von Limonen-Clustern im LTP-Twin-Trap Massenspektrometer Untersuchungen zu den unimolekularen und stoßaktivierten Fragmentierungsmechanismen der Diethyltoluidine über Isotopenmarkierungen Wellenlängenabhängige Photofragmentierung von fluoreszierenden Farbstoffen in einem FT-ICR Massenspektrometer
Gruber, Uschi	caprotec bioanalytics GmbH	Metal labelling of tri-functional Capture Compounds (CCs) to detect protein targets of small molecules
Grübner, Isabell	Goethe Universität Frankfurt, Deutschland	Characterizing the LILBID ionization method: energy transfer and dissociation
Grutters, Michiel	Netherlands Forensic Institute, Forensic Chemistry – Chemical Identification Analysis, 2497 GB The Hague, Netherlands	Development and implementation of new analytical methods and databases for the detection of additives in fuels and fire debris.
Grützmacher, Hans-Friedrich	Department of Chemistry, Bielefeld University	2-Benzylindane radical cations in the gas phase (I): Substituent effects on a stereoselective McLafferty reaction and related hydrogen transfer processes 2-Benzylindane radical cations in the gas phase (II): Substituenteffects on regio- and stereoselective progressive hydrogen scramblingoccurring prior to unimolecular fragmentation
Güttler, Bernd	Physikalisch-Technische-Bundesanstalt, Deutschland	Precise quantification of HIV proteins by isotope dilution mass spectrometry (ID-MS) for applications in HIV diagnostics
Habchi, Johnny	University of Cambridge, United Kingdom	Steps towards a more native analysis of Aß42 using LILBID mass spectrometry
Hachenberger, Yves U.	Humboldt-Universität zu Berlin	Modifikation von Papiersubstraten mit hydrophoben Barrieren zur Erhöhung der Empfindlichkeit und Reproduzierbarkeit in der papierbasierten Massenspektrometrie Vortragend
Hachmöller, Oliver	Institute of Inorganic and Analytical Chemistry, University of Münster, Münster, Germany	Elemental Bioimaging by LA-ICP-QQQ-MS for the Investigation of Wilson´s Disease Vortragend
Hädener, Marianne	University of Bern, Institute of Forensic Medicine, Forensic Toxicology and Chemistry, Bühlstrasse 20, 3012 Bern, Switzerland	Separation of isomeric cannabinoids by high-resolution ion mobility-MS for the differentiation of legal and illegal marijuana Vortragend
Hage, Christoph	Martin-Luther-Universität Halle-Wittenberg, Deutschland	Dissociation behavior of a TEMPO-benzyl cross-linker for peptide structure analysis by free radical initiated peptide sequencing (FRIPS) in negative ESI-MS Vortragend Synthesis of Isotope-Labeled Derivatives of the MS/MS-Cleavable Urea-Cross-Linker: Synthesis and Evaluation of Reactivity for Effective Protein Structure Analysis
Hagenhoff, Sebastian	Westfälische Wilhelms-Universität Münster	Analyse des Peroxid-basierten Sprengstoffs TATP und strukturell verwandter Verbindungen mittels dielektrisch behinderter Entladungsionisations-Massenspektrometrie (DBDI-MS) Vortragend
Hahm, Heung Sik	Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Potsdam, Deutschland	Glycan Fingerprinting using Cold-Ion Infrared Spectroscopy
Hahn, Bill	PerkinElmer LAS (Germany) GmbH, Deutschland	Rapid On Site Analysis of BTX with Portable GC/MS
Hahn, Stefanie	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	The role of mass spectrometry in the identification of autoantigens as targets in neurological autoimmune diseases

Autor(en)	Organisation(en)	Titel des Beitrags
Hahn, Uwe	Universidad Autónoma de Madrid, Spain; University of Strasbourg and CNRS, European School for Chemistry, Polymers and Materials (ECPM), France	Aggregation of a crown-ether decorated zinc-phthalocyanine by collision-induced desolvation providing insight into the electrospray mechanism
Hakelberg, Matthias	caprotec bioanalytics GmbH	Metal labelling of tri-functional Capture Compounds (CCs) to detect protein targets of small molecules
Hamester, Meike	Bruker Daltonik GmbH, Germany	Ultra High Throughput Drug Discovery Screening by MALDI-TOF Mass Spectrometry
Han, Wei	Department of Chemistry, University of Alberta, Edmonton, Canada	Enabling High-Confidence Human Endogenous Metabolite Identification via High-Resolution MS/MS Retention-Time Library
Hann, Stephan	BOKU Wien, Österreich	Standardised Collision Cross Section Measurements by Single Static Drift Field Ion Mobility Instrument in an Interlaboratory Study
Hannich, Thomas	University of Geneva, Department of Biochemistry	Differentiating wild and mutant C. elegans using high-resolution atmospheric pressure matrix assisted laser desorption/ionization mass spectrometry imaging
Hansen, Nils-Owe	Max Planck Institute for the Structure and Dynamics of Matter	Application of laser ablation for tissue metabolomics Lipidomics of Pig Brain Using the PIRL-DIVE Homogenisation Technique Proteomic investigation of skin cell layers by tissue ablation using picosecond infrared laser (PIRL) Sampling of tissues with the picosecond-infrared-laser ablation for Redox Proteomics
Hansman, Grant	DKFZ and Department of Infectious Diseases and Virology University of Heidelberg, Heidelberg, Germany	Studying viral capsid glycan interaction with native MS
Hardy, Neil	Departments of Platform Technology & Science, GlaxoSmithKline, Stevenage, UK	Ultra High Throughput Drug Discovery Screening by MALDI-TOF Mass Spectrometry
Hart, Philippa J.	Waters Corporation, United Kingdom	Getting DESI Imaging up to speed for clinical applications
Hartmann, Laura	Institute for Organic and Macromolecular Chemistry Heinrich-Heine-University Düsseldorf, Düsseldorf Germany	Native mass spectrometry analysis of norovirus - glycan mimetics interaction
Haslam, Carl	Departments of Platform Technology & Science, GlaxoSmithKline, Stevenage, UK	Ultra High Throughput Drug Discovery Screening by MALDI-TOF Mass Spectrometry
Hayen, Heiko	Westfälische Wilhelms-Universität Münster	Analyse des Peroxid-basierten Sprengstoffs TATP und strukturell verwandter Verbindungen mittels dielektrisch behinderter Entladungsionisations-Massenspektrometrie (DBDI-MS) Profiling von konfigurationsisomeren Phospholipiden mittels HILIC-ESI-MS/MS Bestimmung von Doppelbindungspositionen in Lipiden mittels photochemischer Nachsäulenderivatisierung und Tandem-MS
Hayen, Heiko	WWU Münster, Deutschland	Online SPE-HILIC-ESI-MS/MS zur Untersuchung des Metabolismus von auf Acetyl-CoA und Malonyl-CoA in MCF-7 Brustkrebszellen
Heber, Volker	PerkinElmer, Deutschland	Combined Fast Mode and Polarity Switching for Analysis of a Range of Vitamins and Nutritional Supplements in a Single Injection Vortragend
Heck, Albert	Universiteit Utrecht, The Netherlands	Optimization of crosslinked peptide analysis on an Orbitrap Fusion Lumos mass spectrometer
Heemskerk, Johan W. M.	Department of Biochemistry, Cardiovascular Research Institute Maastricht, Maastricht University, The Netherlands;	Temporal quantitative phosphoproteomics of ADP stimulation reveals novel central nodes in platelet activation and inhibition
Heeren, Ron M.A.	Maastricht University, Niederlande	Translational mass spectrometry: Molecular images and more. Vortragend
Heidemann, Johannes	Heinrich-Pette-Institut, Hamburg, Deutschland; Heinrich-Pette-Institute, Leibniz Institute for	Analyzing self-assembly of Ebola virus nucleoprotein with native mass spectrometry Structural characterization of protein-lipid complexes involved in clathrin-mediated endocytosis Vortragend

Autor(en)	Organisation(en)	Titel des Beitrags
	Experimental Virology, Hamburg, Germany	
Heikaus, Laura	University Medical Center Hamburg-Eppendorf, Deutschland	Application of laser ablation for tissue metabolomics
Heikaus de Figueiredo, Laura	University Medical Center Hamburg Eppendorf, Deutschland	Proteome-wide detection of proteolysis in blood plasma by the SDS-PAGE-migration profile Vortragend
Heiles, Sven	Institute of Inorganic and Analytical Chemistry, Justus-Liebig-University, Giessen, Germany	Charge Switching of Phospholipids using Paternó-Büchi Reactions Implementation of Ultraviolet Photodissociation on a LTQ FT Ultra Mass Spectrometer and first Applications Vortragend Reactive low temperature plasma (LTP) mass spectrometry of neurosteroids
Heiling, Sven	Max Planck Institute for Chemical Ecology, Department for Molecular Ecology, Jena, Germany	Metabolomics to study the “war” between plants and insects - Systemic defense induction and post-ingestive rearrangement of plant toxins in insects.
Heimerl, Jule	Humboldt-Universität zu Berlin, Institut für Chemie, Deutschland	A new internal standard approach for laser ablation ICP-MS of polyacrylamide gels
Heintze, Christoph	B-CUBE Center for Molecular Bioengineering, Dresden, Deutschland	Polyamine modifications in biosilica-associated proteome
Helle, Niklas	Universität Kiel, Deutschland	REMPI- und MATI-Spektroskopie an den Methylpyridinen Vortragend
Hellwig, Nils	Institut für Physikalische und Theoretische Chemie, Goethe-Universität Frankfurt; Goethe-University Frankfurt/Main, Deutschland	From Salty to Salt-free: Monitoring the Salt-dependent Dissoziation of the Membrane Protein Complex GCD in a Single Experiment Vortragend Monitoring and correlating of protein charge states with respect to amino acid modification and buffer conditions
Hempel, Ute	Institute of Physiological Chemistry, Faculty of Medicine Carl Gustav Carus, Technical University Dresden, Germany	Comparative analysis of the effects of sulfated hyaluronic acid and dexamethasone on osteoblast differentiation by nanoLC-MS and random forest modeling.
Hendgen-Cotta, Ulrike B.	University Hospital Essen, Medical Faculty, West German Heart and Vascular Center, Department of Cardiology and Department of Angiology, Germany	SIMPLEX reveals myoglobin as a key player in cardiac lipid metabolism
Hendrikse, Jeanet	Netherlands Forensic Institute, Forensic Chemistry – Chemical Identification Analysis, 2497 GB The Hague, Netherlands	Development and implementation of new analytical methods and databases for the detection of additives in fuels and fire debris.
Henkel, Corinna	Bruker Daltonik GmbH, Bremen, Germany	2ω-FT-ICR Mass Spectrometry with Quadrupolar Detection
Henrion, André	Physikalisch-Technische-Bundesanstalt, Deutschland	Precise quantification of HIV proteins by isotope dilution mass spectrometry (ID-MS) for applications in HIV diagnostics
Hense, Genia	Goethe Universität Frankfurt, Deutschland	Characterizing the LILBID ionization method: energy transfer and dissociation
Herfurth, Uta M.	Universität Leipzig, Fakultät für Chemie und Mineralogie, Germany	Probing plant Maillard reaction by mass spectrometry in model peptide systems
Hinz, Klaus Peter	Justus-Liebig Universität Giessen, Deutschland	Resolution enhancement by delayed ion extraction in a single-particle aerosol mass spectrometer Optimization of the LAMPAS 3 laser mass spectrometer for improved on-line single particle analysis Vortragend
Hirtz, Christophe	Laboratoire de Biochimie et Protéomique Clinique, Institut de Médecine Régénératrice et de Biothérapie, CHU de Montpellier - Hôpital St. Eloi, Montpellier, France	Applying a Proteoform profiling method for neurological disorder biomarker discovery operations
Hitzenberger, Jakob F.	Friedrich-Alexander Universität Erlangen-Nürnberg, Deutschland	Formate attachment to ZnPorphyrin- and ZnPhthalocyanine-Oligomers: Binding, Fragmentation, Affinity Reactivity and stability check of even vs. odd electron (quasi)-molecular ions derived from triangulenium type derivatives Vortragend

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Hoehenwarter, Wolfgang	Proteome Analytics Research Group, Leibniz Institute of Plant Biochemistry	Simulated microgravity triggers transient enhancement of protein glycation and oxidation in germinating Brassica napus seeds
Hoffmann, Christian	Free Floater (Junior) Research Group Applied Synthetic Biology, Georg-August University Göttingen, Institute for Microbiology and Genetics, 37077 Göttingen, Germany	Partial Immunoblotting of 2D-Gels: A Novel Method to Identify Post-Translationally Modified Proteins Exemplified for the Myelin Acetylome
Hoffmann, Jan	University of Frankfurt, Deutschland	Applications of non-covalently bound membrane proteins in nanodiscs using LILBID-MS Monitoring and correlating of protein charge states with respect to amino acid modification and buffer conditions
Hoffmann, Ralf	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig, Germany; Center for Biotechnology and Biomedicine, Universität Leipzig, Germany	Identification of oxidative biomarkers in synovial fluid of patients suffering from rheumatoid arthritis Protein carbonylation in raw milk and differently processed milk products
Hoffmann, Waldemar	Freie Universität Berlin; Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin	Investigation of Dimeric and Hexameric Halogen-Bonded Supramolecular Capsules by ESI-MS and IM-MS The Amyloid Formation Mechanism of Human IAPP: An Infrared Spectroscopy Approach Vortragend Glycan Fingerprinting using Cold-Ion Infrared Spectroscopy
Hofmann, Diana	Forschungszentrum Jülich, Deutschland	Historical charcoal additions potentially improve stability of soil organic carbon Vortragend
Hofmann, Tommy	Interdisciplinary research center HALOmem, Martin Luther University Halle-Wittenberg, Kurt-Moses-Straße-3, 06120 Halle (Saale).; Helmholtz-Centre for Environmental research (UFZ), Department of Molecular Systems Biology, Leipzig, Germany; HALOmem, Halle (Saale), Germany	Fragmentation behavior of neuronal lipids by HCD-MS/MS Vortragend Phthalate metabolites MEHP and MEOHP but not the phthalate DEHP itself bind and activate the PPARγ
Holterhus, Paul-Martin	Universitätsklinikum Schleswig-Holstein, Deutschland	Entwicklung einer LC-MS/MS Methode zur Bestimmung der Backdoorpathway Hormone Androsterone und Androstandiol und der Androgene Androstendion, Testosteron und Dihydrotestosteron
Hooton, Kevin	Department of Chemistry, University of Alberta, Edmonton, Canada	Enabling High-Confidence Human Endogenous Metabolite Identification via High-Resolution MS/MS Retention-Time Library
Horner, Gerhard	Five Technologies GmbH, Frauenstrasse 22, 80469 Munich, Germany	FAST MULTIPLEXING OF IONISATION ENERGY FOR PERFORMANCE IMPROVEMENTS IN GC-TOF MS Vortragend
Hoyes, John	Waters Corporation, Wilmslow, United Kingdom	Quantitation of Proteomics Samples Using a Novel Scanning Quadrupole DIA Method
Hübner, Florian	Institute of Food Chemistry, University of Münster, Germany	Algorithms for the annotation of isotopes, fragments and adducts, applied to HPLC-HRMS metabolomics data for the discovery of novel compounds
Hughes, Chris	Waters Corporation, Wilmslow, United Kingdom	Lipidomics Quantitation Using a Novel Scanning Quadrupole DIA Method Quantitation of Proteomics Samples Using a Novel Scanning Quadrupole DIA Method
Humpf, Hans-Ulrich	Institute of Food Chemistry, University of Münster, Germany	Algorithms for the annotation of isotopes, fragments and adducts, applied to HPLC-HRMS metabolomics data for the discovery of novel compounds Localization of Ergot Alkaloids in Sclerotia of Claviceps purpurea by MALDI-MS Imaging
Hunger, Doreen	2Department of Microbiology, Institute of Biology, Martin-Luther University Halle-Wittenberg, Halle (Saale), Germany	Mass Spectrometry-Based Interaction Studies of the N-Terminus of the Formate Channel FocA from Escherichia coli
Hunter, Christie	SCIEX, USA	Accelerating Data Independent Acquisition with Microflow Chromatography

Autor(en)	Organisation(en)	Titel des Beitrags
Hutterli, Manuel	TOFWERK, Schweiz	Characterization of a New Extractive Electrospray Ionization (EESI) Source for Online Particle Analysis and its Application to Atmospheric Aerosol
Iacobucci, Claudio	UMR CNRS 6521, Université de Bretagne Occidentale, 6 Av.Le Gorgeu, 29200 Brest, France; Institute of Pharmacy, Martin-Luther University Halle-Wittenberg, Halle/Saale, Germany, Deutschland	COPPER-CATALYSED CLICK REACTION PERFORMED IN THE GAS PHASE: A COMBINED MASS SPECTROMETRIC AND DFT MECHANISTIC STUDY Vortragend
Ickert, Stefanie	Bundesanstalt für Materialforschung- und prüfung, Deutschland	Collision Specific Fragmentation of Oligonucleotides in Tandem Mass Spectrometry Experiments Vortragend
Ihling, Christian	Martin-Luther Universität Halle-Wittenberg, Institute of Pharmacy; Institute of Pharmacy, Martin Luther University Halle-Wittenberg; Martin-Luther-University Halle-Wittenberg, Institute of Pharmacy, Department of Pharmaceutical Chemistry and Bioanalytics, Germany	Age-related formation of advanced glycation end products (AGEs) in root nodules of common beans (Phaseolus vulgaris) An Integrated Mass Spectrometry Based Approach to Probe the Structure of the Full-Length Wild-Type Tetrameric p53 Tumor Suppressor An Integrated Workflow for Structural Proteomics Studies based on Cross-linking/Mass Spectrometry with an MS/MS Cleavable Cross-linker Vortragend Cross-Linking and Mass Spectrometry Shed New Light on the bMunc13-2/Calmodulin Interaction Simulated microgravity triggers transient enhancement of protein glycation and oxidation in germinating Brassica napus seeds Structural Insights into Retinal Guanylyl Cyclase/GCAP-2 Interaction by Cross-linking and Mass Spectrometry
Ivanović-Burmacović, Ivana	Friedrich-Alexander-University Erlangen-Nürnberg, Deutschland	Aggregation of a crown-ether decorated zinc-phthalocyanine by collision-induced desolvation providing insight into the electrospray mechanism
Jahn, Olaf	Max-Planck-Institut für Experimentelle Medizin, Göttingen, Deutschland; Center for Nanoscale Microscopy and Molecular Physiology of the Brain, 37075 Göttingen, Germany	Cross-Linking and Mass Spectrometry Shed New Light on the bMunc13-2/Calmodulin Interaction Following the Unfolding and Dissociation of Calmodulin/Munc13 Complexes by Ion Mobility-Mass Spectrometry Partial Immunoblotting of 2D-Gels: A Novel Method to Identify Post-Translationally Modified Proteins Exemplified for the Myelin Acetylome Vortragend
Jahnke, Siegfried	IBG-2 Pflanzenwissenschaften, Forschungszentrum Jülich, Deutschland	Quantitative turnover analysis of chlorophylls, carotenoids and tocopherol in green leaves by LC-MS and FTICR-MS
Jakimovska, Viktorija	Ss. Cyril and Methodius University of Skopje, Republic of Macedonia	Methodological aspects of mass spectrometric detection for profiling ambient VOCs with thermodesorption-GCMS
Jakubowski, Norbert	Bundesanstalt für Materialforschung und -prüfung, Berlin	Mass Spectrometry Imaging as Tool for the Analysis of MRI Contrast Agents in Biological Tissues
Janzik, Ingar	IBG-2 Pflanzenwissenschaften, Forschungszentrum Jülich, Deutschland	Quantitative turnover analysis of chlorophylls, carotenoids and tocopherol in green leaves by LC-MS and FTICR-MS
Jeck, Viola	Westfälische Wilhelms-Universität Münster, Deutschland	Bestimmung von Doppelbindungspositionen in Lipiden mittels photochemischer Nachsäulenderivatisierung und Tandem-MS Vortragend
Jeibmann, Astrid	University Hospital of Münster, Institute of Neuropathology, Münster, Germany	Bioimaging of photosensitizers in human brain tumors after fluorescence-guided resection
Jertz, Roland	Bruker Daltonik GmbH, Bremen, Germany	2ω-FT-ICR Mass Spectrometry with Quadrupolar Detection MALDI FT-ICR Imaging: Double the Performance or Double the Samples using Quadrupolar Detection
John, Harald	Bundeswehr Institute of Pharmacology and Toxicology	Albumin adducts as biomarkers of an exposure with organophosphorus pesticides Mass spectrometric investigation of N acetylcysteine as a potential scavenger against sulfur mustard
Jones, Emrys	Waters Corporation, United Kingdom	Getting DESI Imaging up to speed for clinical applications
Joseph, Shai R	Max Planck Institute of Molecular Cell Biology and	Absolute quantification of core histones in zebrafish embryos by MS Western

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	Genetics, Dresden, Germany, Deutschland	
Josephs, Jonathan	Thermo Fisher Scientific, USA	Full Characterization of Antibodies Under Denaturing and Native Conditions on a Hybrid Quadrupole-Orbitrap MS Equipped With a Higher Mass Range
Jurk, Kerstin	Center for Thrombosis and Hemostasis, Universitätsklinikum der Johannes Gutenberg-Universität Mainz, Mainz, Germany;	Temporal quantitative phosphoproteomics of ADP stimulation reveals novel central nodes in platelet activation and inhibition
Kade, Stephanie	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	The role of mass spectrometry in the identification of autoantigens as targets in neurological autoimmune diseases
Kadesch, Patrik	Justus-Liebig-Universität Gießen, Institut für Anorganische und Analytische Chemie	AP-SMALDI MSI of metabolites and lipids in Schistosoma mansoni parasites Vortragend
Kaefer, Uwe	Cooperation Group ''Comprehensive Molecular Analytics", Helmholtz Zentrum Muenchen, Munich, GERMANY	The Usage of Direct Inlet Probe in combination with High Resolution Mass Spectrometry
Käfer, Uwe	Helmholtz Zentrum Muenchen, Neuherberg	The Usage of Direct Inlet Probe in combination with High Resolution Mass Spectrometry for the Characterization of Heavy Petroleum Products Vortragend
Kaftan, Filip	Max Planck Institute for Chemical Ecology, Jena, Germany	Application of the Superbasic Matrix DPN in Atmospheric Pressure MALDI-MS-Analyses of Biological Samples
Kaleja, Patrick	AG Systematische Proteomforschung & Bioanalytik, Institut für Experimentelle Medizin, Christian-Albrechts-Universität, Kiel; Klinik für Unfallchirurgie und Traumatologie, Experimentelle Unfallchirurgie, UKSH, Kiel	Quantitative proteomics for the analysis of molecular changes in lung adenocarcinoma cells in response to Vitamin D3 Vortragend
Kalinowski, Jörn	Bielefeld University, Bielefeld, Deutschland	Boosting compound identification confidence in Metabolomics by exploiting all available Q-TOF high resolution accurate mass spectral information.
Kalkhof, Stefan	Department of Bioanalytics, University of Applied Sciences of Coburg, Germany; Helmholtz-Centre for Environmental research (UFZ), Department of Molecular Systems Biology, Leipzig, Germany	Comparative analysis of the effects of sulfated hyaluronic acid and dexamethasone on osteoblast differentiation by nanoLC-MS and random forest modeling. Phthalate metabolites MEHP and MEOHP but not the phthalate DEHP itself bind and activate the PPARγ
Kanawati, Basem	Helmholtz Zentrum München, Deutschland	Power-function Resolution Filter in Fourier Transform Mass Spectrometry Vortragend
Kappert, Christin	Max Planck Institute for Biophysical Chemistry, Göttingen, Germany	Analysis of UV-induced DNA–protein cross-links in a chromatin model
Karaköse, Hande	Division of Bioanalytical Chemistry, Research Center Borstel, Germany; German Center for Infection Research, Clinical Tuberculosis Center, Borstel, Germany	LC-MS2 Method Development for Simultaneous Analysis of Antibiotics from Plasma of MDR-TB Patients Vortragend
Karas, Michael	Goethe Universität, Frankfurt, Deutschland	A versatile method to extract, modify, enrich and digest proteomic samples directly from cell lysates CICCA-Tetrazole: An alternative matrix for the analysis of low molecular weight compounds by MALDI-MS ArgC-like digestion: complementary or alternative to tryptic digestion? Investigating on-plate digestion of proteins with regard to trypsin activity and oxidation

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Karimi, Kudratullah	Goethe-University Frankfurt/Main, Deutschland	Monitoring and correlating of protein charge states with respect to amino acid modification and buffer conditions Vortragend
Karst, Uwe	Institute of Inorganic and Analytical Chemistry, University of Münster, Germany; Westfälische Wilhelms-Universität Münster, Deutschland	Algorithms for the annotation of isotopes, fragments and adducts, applied to HPLC-HRMS metabolomics data for the discovery of novel compounds Analysis of Liquid Crystal Display Sealants using Spatially Resolved Mass Spectrometric Methods Automated electrochemistry/mass spectrometry for high-throughput analysis of xenobiotics Bioimaging of photosensitizers in human brain tumors after fluorescence-guided resection Differentiation and Identification of Explosives Formulations by Means of HPLC-MS Electrochemical conversion of Pt(IV) prodrugs to Pt(II) cytostatics investigated by means of liquid chromatography and mass spectrometry Elemental Bioimaging by LA-ICP-QQQ-MS for the Investigation of Wilson´s Disease Imaging of Cerium Oxide Nanoparticles and Phospholipids in Rat Lung Tissue by Means of LA-ICP-MS and MALDI-MS Investigating the zinc distribution in the mayfly N. triangulifer using elemental bioimaging by LA-ICP-MS Investigations on the photolysis of sulfamethoxazole Molecular laser ablation-mass spectrometry for rapid identification of synthetic cannabinoids
Kaspar-Schoenefeld, Stephanie	Bruker Daltonik GmbH, Deutschland	Investigation of Q-TOF instruments advantages for label-free proteome analysis
Kasuch, Sandra	Federal Criminal Police Office, Forensic Institute, 65193 Wiesbaden, Germany	Development and implementation of new analytical methods and databases for the detection of additives in fuels and fire debris.
Kaub, Johannes	Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Deutschland	Optimized Biomolecular Extraction Using Desorption by Impulsive Vibrational Excitation: Applications to Embryonic Cell Differentiation Vortragend
Kellner, Ina	Friedrich-Alexander-University Erlangen-Nürnberg, Deutschland	Aggregation of a crown-ether decorated zinc-phthalocyanine by collision-induced desolvation providing insight into the electrospray mechanism Vortragend
Keppler, Bernhard K.	Universität Wien, Österreich	Electrochemical conversion of Pt(IV) prodrugs to Pt(II) cytostatics investigated by means of liquid chromatography and mass spectrometry
Kessler, Nikolas	Bruker Daltonik GmbH, Deutschland	Boosting compound identification confidence in Metabolomics by exploiting all available Q-TOF high resolution accurate mass spectral information.
Kettling, Hans	University of Münster, Insitute for Hygiene, Münster, Germany; Interdisciplinary Center for Clinical Research (IZKF) Münster, Germany	CoolMALDI: Combination of IR-ablation and UV-postionization of snap-frozen tissue sections for sensitive imaging of lipids and metabolites
Khalil, Saleh mahmud	Justus Liebig University Giessen, Institute of Inorganic and Analytical Chemistry	Differentiating wild and mutant C. elegans using high-resolution atmospheric pressure matrix assisted laser desorption/ionization mass spectrometry imaging Vortragend
Kiani, Parnian	University Medical Centre Hamburg-Eppendorf, Institute for Clinical Chemistry, Department for Mass Spectrometric Proteomics, Hamburg	Proteomic investigation of skin cell layers by tissue ablation using picosecond infrared laser (PIRL) Vortragend
Kim, Ahyoung	Leibniz Institute of Plant Biochemistry, Department of Bioorganic Chemistry; Universität Leipzig, Faculty of Chemistry and Mineralogy	Age-related formation of advanced glycation end products (AGEs) in root nodules of common beans (Phaseolus vulgaris) Vortragend
Kiontke, Andreas	Universität Leipzig, Deutschland	Impact factors on signal response with low temperature plasma ionization for mass spectrometry Vortragend
Kipping, Marc	Waters GmbH, Eschborn, Deutschland	IMS-DIA-MS Characterisation and IMS-MRM QconCAT Quantitation of the Lipidome and Apolipoprotein Complements of Obesity and Diabetes Cohorts Vortragend Quantitation of Proteomics Samples Using a Novel Scanning Quadrupole DIA Method Vortragend

Autor(en)	Organisation(en)	Titel des Beitrags
Kirsch, Dieter	Federal Criminal Police Office, Forensic Institute, 65193 Wiesbaden, Germany	Development and implementation of new analytical methods and databases for the detection of additives in fuels and fire debris.
Kivala, Milan	Friedrich-Alexander-University Erlangen-Nürnberg, Germany	Reactivity and stability check of even vs. odd electron (quasi)-molecular ions derived from triangulenium type derivatives
Klee, Sonja	TOFWERK, Schweiz	Characterization of a New Extractive Electrospray Ionization (EESI) Source for Online Particle Analysis and its Application to Atmospheric Aerosol Vortragend
Klein, Jonas	University Medical Center Hamburg-Eppendorf, Deutschland	Application of laser ablation for tissue metabolomics Vortragend
Kniese, Jasmin	Universität Bayreuth, Deutschland	Multimodal imaging combining mass spectrometry and vibrational spectroscopy using a single tissue section and an integrated data processing workflow
Knochenmuss, Richard	Tofwerk, Uttigenstrasse 22, CH-3600 Thun, Switzerland	Differentiation and relative quantification of chondroitin sulfate isomers by ion mobility spectrometry-mass spectrometry and pulsed-field gradient NMR
Koch, Annika	Institute for Hygiene, University of Münster, Robert-Koch-Str. 41, 48149 Münster, Germany	The internal energy in a MALDI plume probed with thermometer molecules: Effects of laser excitation wavelength and laser fluence
Koch, Annika	University of Münster, Institute of Hygiene, Biomedical Mass Spectrometry, Germany	Colorful MALDI: Effect of the Laser Excitation Wavelength on the Analytical Sensitivity in Standard MALDI-MS and Imaging Experiments Vortragend
Koch, Arne	University of Leipzig, Germany	Methodological aspects of mass spectrometric detection for profiling ambient VOCs with thermodesorption-GCMS
Koch, Winfried	Oil-Wärme-Institut GmbH, Herzogenrath, Deutschland	Thermogravimetry coupled to Ultrafast Gas Chromatography Singlephoton-Ionisation Time-of-Flight-Mass-Spectrometry (TG-SPI-TOF-MS) for Evolved-Gas-Analysis of Fuels regarding to the Deposit Formation Potential
Koellensperger, Gunda	Universität Wien, Österreich	Electrochemical conversion of Pt(IV) prodrugs to Pt(II) cytostatics investigated by means of liquid chromatography and mass spectrometry
Koenig, Stefan	Institute of Forensic Medicine, University of Bern	N-Acetyltaurine as a novel urinary ethanol marker in a drinking study
Köhler, Jörg	Markes International GmbH, Schleussnerstrasse 42, Frankfurt, Germany	FAST MULTIPLEXING OF IONISATION ENERGY FOR PERFORMANCE IMPROVEMENTS IN GC-TOF MS
Köhler, Niklas	Division of Clinical Infectious Diseases, Research Center Borstel, Borstel, Germany; German Center for Infection Research, Clinical Tuberculosis Center, Borstel, Germany	LC-MS2 Method Development for Simultaneous Analysis of Antibiotics from Plasma of MDR-TB Patients
Kokesch-Himmelreich, Julia	Universität Bayreuth, Deutschland	Multimodal imaging combining mass spectrometry and vibrational spectroscopy using a single tissue section and an integrated data processing workflow
Kölbel, Knut	Universiteit Antwerpen, Belgien	Formation and Properties of a Compact Protein Unfolding Intermediate in the Gas-phase Vortragend
Kolter, Marlene	Georg-August-Universität Göttingen, Deutschland	Stability and Unimolecular Reactivity of Organopalladate(II) Complexes Vortragend
Komorowski, Lars	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	The role of mass spectrometry in the identification of autoantigens as targets in neurological autoimmune diseases
Kompauer, Mario	Justus Liebig University Giessen, Germany; Institut für Anorganische und Analytische Chemie; Justus-Liebig-Universität Gießen	Implementation of a High Repetition-Rate Laser System in an AP-SMALDI MSI System for Enhanced Measurement Speed Vortragend Implementation of Ultraviolet Photodissociation on a LTQ FT Ultra Mass Spectrometer and first Applications
Kondyli, Aikaterini	Max Planck Institut für Kohlenforschung, Germany	Effect of temperature on crude oil fouling under inert and oxygenated conditions and subsequent analysis by HRMS Vortragend
Konietzny, Rebecca	Agilent Technologies, Waldbronn, Deutschland	Standardised Collision Cross Section Measurements by Single Static Drift Field Ion Mobility Instrument in an Interlaboratory Study
König, Simone	WWU Münster	Pyrylium-based dye and charge tagging in proteomics
König, Vanessa	Hochschule Mannheim, Deutschland	Derivatization of low-volatile compounds in aqueous solution and analysis by HS-GC-IMS

Autor(en)	Organisation(en)	Titel des Beitrags
Kopczynski, Dominik	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Germany	A new bridge between targeted and non-targeted LC-MS/MS lipidomics PeptideMapper: Efficient and Versatile Amino Acid Sequence and Tag Mapping Vortragend
Kopicki, Janine	Heinrich-Pette-Institut, Hamburg, Deutschland	Analyzing self-assembly of Ebola virus nucleoprotein with native mass spectrometry Vortragend
Koschinski, Stefan	Markes International GmbH, Schleussnerstrasse 42, Frankfurt, Germany	FAST MULTIPLEXING OF IONISATION ENERGY FOR PERFORMANCE IMPROVEMENTS IN GC-TOF MS
Köster, Claus	Bruker-Daltonik GmbH, Bremen	Untersuchung von Limonen-Clustern im LTP-Twin-Trap Massenspektrometer
Koszinowski, Konrad	Georg-August-Universität Göttingen, Institut für Organische und Biomolekulare Chemie	Constitution and gas phase reactivity of organocobaltates Stability and Unimolecular Reactivity of Organopalladate(II) Complexes
Koszinowski, Konrad	Institut für Organische und Biomolekuare Chemie, Georg-August-Universität Göttingen, Deutschland; Georg-August-University Göttingen, Germany	An improved approach for calculating dissociation rates of benzylpyridinium ions Coinage-Metal Ate Complexes – An ESI-MS Study Direct Observation and Reactivity Studies of Organoferrates by Electrospray Ionization Mass Spectrometry Internal energy of ions produced by electrospray and cryospray ionization Vortragend
Kowol, Christian R.	Universität Wien, Österreich	Electrochemical conversion of Pt(IV) prodrugs to Pt(II) cytostatics investigated by means of liquid chromatography and mass spectrometry
Kozlov, Ilya	University of Leipzig, Germany	Methodological aspects of mass spectrometric detection for profiling ambient VOCs with thermodesorption-GCMS
Kraj, Agnieszka	ANTEC, Leyden	In situ monitoring of lipid oxidation using electrochemistry-mass spectrometry coupling
Krajewski, Matthias	Division of Bioanalytical Chemistry, Research Center Borstel, Parkallee 10, Borstel, Germany	Software platform to improve the quality control of Lipid mediator quantification
Kramer, Katharina	Max Planck Institute for Plant Breeding Research, Köln, Germany	Analysis of UV-induced DNA–protein cross-links in a chromatin model
Kratochvil, Isabel	Helmholtz-Centre for Environmental research (UFZ), Department of Molecular Systems Biology, Leipzig, Germany	Phthalate metabolites MEHP and MEOHP but not the phthalate DEHP itself bind and activate the PPARγ Vortragend
Kraus, Johanna	Fort Collins Science Center, US Geological Survey, Fort Collins, USA	Investigating the zinc distribution in the mayfly N. triangulifer using elemental bioimaging by LA-ICP-MS
Krause, Eberhard	Leibniz Institut für Molekulare Pharmakologie, Deutschland	Analysis of serine-phosphorylation dependent protein-protein interactions of the T cell adaptor protein ADAP Neutral loss-triggered EThcD mass spectrometry identifies protein pyrophosphorylation in vivo
Kreyenschmidt, Friedrich	Georg-August-Universität Göttingen, Institut für Organische und Biomolekulare Chemie	Constitution and gas phase reactivity of organocobaltates Vortragend Internal energy of ions produced by electrospray and cryospray ionization
Kriete, Claudia	Bruker Daltonik GmbH, Bremen, Germany	2ω-FT-ICR Mass Spectrometry with Quadrupolar Detection MALDI FT-ICR Imaging: Double the Performance or Double the Samples using Quadrupolar Detection
Kröger, Nils	B-CUBE Center for Molecular Bioengineering, Dresden, Deutschland; Department of Chemistry and Food Chemistry, Technische Universität Dresden, Deutschland	Polyamine modifications in biosilica-associated proteome
Kröger, Sabrina	University of Münster, Institute of Inorganic and Analytical Chemistry, Münster, Germany	Bioimaging of photosensitizers in human brain tumors after fluorescence-guided resection Vortragend
Krösser, Dennis	University Medical Center Hamburg-Eppendorf, Deutschland	Comparison of label free quantification methods for proteomics Vortragend Mass spectrometric characterization of aberrant O-glycosylation in COSMC deficient mouse pancreas tissue

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Krüger, Sascha	Universität Kiel, Deutschland	REMPI- und MATI-Spektroskopie an den Methylpyridinen
Kruth, Claudia	Universität Rostock, Deutschland	Direct resonance-enhanced multi-photon ionisation (REMPI) of complex liquid samples under vacuum conditions
Kuballa, Juergen	GALAB Laboratories GmbH, Deutschland	Differentiation of organic and conventional farming of tomatoes by non-targeted metabolomic profiling using travelling-wave ion mobility high resolution mass spectrometry
Kuballa, Jürgen	GALAB Laboratories GmbH, Deutschland	Discrimination of apple and potato cultivars by non-targeted metabolomic fingerprinting via UPLC-IMS-QToF analysis
Kuck, Dietmar	Department of Chemistry, Bielefeld University	2-Benzylindane radical cations in the gas phase (I): Substituent effects on a stereoselective McLafferty reaction and related hydrogen transfer processes Vortragend 2-Benzylindane radical cations in the gas phase (II): Substituenteffects on regio- and stereoselective progressive hydrogen scramblingoccurring prior to unimolecular fragmentation Vortragend
Kücklich, Marlen	Universität Leipzig, Deutschland	The performance of mobile GC-MS for field sampling of body odours from common marmosets (Callithrix jacchus)
Kugler, Christian	LungenClinic Großhansdorf, Wöhrendamm 80, 22927 Großhansdorf.	Lipidomes of human lung tissues show distinct lipid metabolic alterations for lung cancer and pulmonary emphysema
Kühne, Stephan	Bruker Daltonik GmbH, Deutschland	A step forward in GC-HRAM-MS based metabolomics - A novel atmospheric pressure GC-APCI Source increases quantitative and qualitative performance Vortragend Enabling High-Confidence Human Endogenous Metabolite Identification via High-Resolution MS/MS Retention-Time Library Vortragend
Kukačka, Zdeněk	Steinbeis Center for Biopolymer Analysis and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany	Innovative analytical methodologies for the development of new antitubercular agents
Kulkarni, Purva	Max Planck Institute for Chemical Ecology, Jena, Germany; Lehrstuhl für Bioinformatik, Friedrich Schiller University, Jena, Germany; Research Group Mass spectrometry/Proteomics, Max Planck Institute for Chemical Ecology	Application of high-throughput MS screening to disentangle the bacterial metabolome Mapping metabolites from rough terrain: laser ablation electrospray ionization on non-flat samples
Kulle, Alexandra	Universitätsklinikum Schleswig-Holstein, Deutschland	Entwicklung einer LC-MS/MS Methode zur Bestimmung der Backdoorpathway Hormone Androsterone und Androstandiol und der Androgene Androstendion, Testosteron und Dihydrotestosteron Vortragend
Kumar, Mukesh	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany, Deutschland	Absolute quantification of core histones in zebrafish embryos by MS Western Vortragend
Kuo, Alex	Academia Sinica, School of Chemistry, Taipei, Taiwan	Increased confidence for the identification of N-linked glycopeptides using an optimised collision energy workflow
Kurulugama, Ruwan	Agilent Technologies, Santa Clara, USA	Standardised Collision Cross Section Measurements by Single Static Drift Field Ion Mobility Instrument in an Interlaboratory Study
Kusch, Kathrin	Department of Neurogenetics, Max-Planck-Institute of Experimental Medicine, 37075 Göttingen, Germany	Partial Immunoblotting of 2D-Gels: A Novel Method to Identify Post-Translationally Modified Proteins Exemplified for the Myelin Acetylome
Kuzmich, Oleksandra	Humboldt Universität zu Berlin, Deutschland	Metal labelling of tri-functional Capture Compounds (CCs) to detect protein targets of small molecules Vortragend
Kwiatkowski, Marcel	University Medical Center Groningen, Department of Pulmonary Diseases and Tuberculosis, Groningen, The Netherlands.; University of Groningen, Department of Analytical Biochemistry, The Netherlands.	Mass Spectrometric Characterization of Proteins from condensates of the Picosecond Infrared Laser Ablation Vortragend
Kwiatkowski, Marcel	Mass Spectrometric Proteomics, Department of	Sampling of tissues with the picosecond-infrared-laser ablation for Redox Proteomics

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	Clinical Chemistry, University Medical Center Hamburg-Eppendorf, Hamburg, Germany.	
Lang, Johannes	II physikalisches Insitut, Justus-Liebig-Universität Gießen, Deutschland	Tandem Mass Spectrometry with a (Ultra-)High Resolving Time-of-Flight Mass Spectrometer
Lange, Christoph	Division of Clinical Infectious Diseases, Research Center Borstel, Borstel, Germany; German Center for Infection Research, Clinical Tuberculosis Center, Borstel, Germany; International Health/Infectious Diseases, University of Lübeck, Lübeck, Germany	LC-MS2 Method Development for Simultaneous Analysis of Antibiotics from Plasma of MDR-TB Patients
Lange, Mike	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig; Center for Biotechnology and Biomedicine, Universität Leipzig, Germany	oxLipidomics data integration for systems medicine view on metabolic diseases
Lange, Tobias	University Medical Center Hamburg-Eppendorf, Deutschland	Comparison of label free quantification methods for proteomics
Langer, Julian	MPI for Biophysics, Frankfurt am Main, GERMANY	SelexION® DMS-based detergent interference removal for shotgun-lipidomics analyses
Langridge, James	Waters Corporation, Wilmslow, United Kingdom	Lipidomics Quantitation Using a Novel Scanning Quadrupole DIA Method IMS-DIA-MS Characterisation and IMS-MRM QconCAT Quantitation of the Lipidome and Apolipoprotein Complements of Obesity and Diabetes Cohorts Quantitation of Proteomics Samples Using a Novel Scanning Quadrupole DIA Method
Lebon, Alexandre	UMR CNRS 6521, Université de Bretagne Occidentale, 6 Av.Le Gorgeu, 29200 Brest, France	COPPER-CATALYSED CLICK REACTION PERFORMED IN THE GAS PHASE: A COMBINED MASS SPECTROMETRIC AND DFT MECHANISTIC STUDY
Lee, Hee-Jin	Humboldt-Universität zu Berlin, Deutschland	Mass Spectrometry Imaging as Tool for the Analysis of MRI Contrast Agents in Biological Tissues
Lehmann, Sylvain	Laboratoire de Biochimie et Protéomique Clinique, Institut de Médecine Régénératrice et de Biothérapie, CHU de Montpellier - Hôpital St. Eloi, Montpellier, France	Applying a Proteoform profiling method for neurological disorder biomarker discovery operations
Lehmann, Wolf-Dieter	Biochemie-Zentrum Heidelberg, Deutschland; DKFZ Heidelberg; Deutsches Krebsforschungszentrum (DKFZ) Heidelberg	Quantitative Positional Isomer Analysis of Mixed Diacyl-Glycerophospholipids (dGPLs) by Ultra Performance Liquid Chromatography-Electrospray-Tandem Mass Spectrometry (UPLC-ESI-MS/MS) Spotting of Structural Isomer Mixtures of Diacyl-Glycerophospholipids via UPLC-MS/MS Vortragend
Leipert, Jan	AG Systematische Proteomforschung & Bioanalytik, Institut für Experimentelle Medizin, Christian-Albrechts-Universität zu Kiel, Kiel, Deutschland	Identification and quantification of N-acyl homoserine lactones involved in bacterial communication by matrix-assisted laser desorption/ionization mass spectrometry Vortragend
Lemesheva, Valeriia	St-Petersburg State University, Russia	Application of LC-MS technique for intra-thallus profiling of polyphenolics in three species of fucoid algae
Lemmnitzer, Katharina	University of Leipzig, Medical Faculty, Institute of Medical Physics and Biophysics	Differentiation and relative quantification of chondroitin sulfate isomers by ion mobility spectrometry-mass spectrometry and pulsed-field gradient NMR Vortragend
Lenz, Thomas	caprotec bioanalytics GmbH	Metal labelling of tri-functional Capture Compounds (CCs) to detect protein targets of small molecules
Leonhard, Peter	Merck KGaA, Frankfurter Str. 250, 64293 Darmstadt, Germany	Analysis of Liquid Crystal Display Sealants using Spatially Resolved Mass Spectrometric Methods

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Leveridge, Melanie	Departments of Platform Technology & Science, GlaxoSmithKline, Stevenage, UK	Ultra High Throughput Drug Discovery Screening by MALDI-TOF Mass Spectrometry
Lewin, Yannik	Goethe Universität, Frankfurt, Deutschland	A versatile method to extract, modify, enrich and digest proteomic samples directly from cell lysates Vortragend
Li, Bin	Department of Chemistry, University of Illinois, 405 North Mathews Avenue, 61801 Urbana, Illinois, USA	Imaging metabolites in wheat stem base-Fusarium graminearum interactions using high-resolution atmospheric pressure scanning microprobe MALDI mass spectrometry imaging (SMALDI-MSI)
Li, Liang	Department of Chemistry, University of Alberta, Edmonton, Canada	Enabling High-Confidence Human Endogenous Metabolite Identification via High-Resolution MS/MS Retention-Time Library
Li, Yan	Helmholtz Zentrum München, Deutschland	Power-function Resolution Filter in Fourier Transform Mass Spectrometry
Li, Zhendong	Department of Chemistry, University of Alberta, Edmonton, Canada	Enabling High-Confidence Human Endogenous Metabolite Identification via High-Resolution MS/MS Retention-Time Library Enabling High-Confidence Human Endogenous Metabolite Identification via High-Resolution MS/MS Retention-Time Library
Lieblein, Tobias	Goethe-Universität Frankfurt, Deutschland	Steps towards a more native analysis of Aß42 using LILBID mass spectrometry Vortragend
Liepold, Thomas	Proteomics Group, Max-Planck-Institute of Experimental Medicine, 37075 Göttingen, Germany	Partial Immunoblotting of 2D-Gels: A Novel Method to Identify Post-Translationally Modified Proteins Exemplified for the Myelin Acetylome
Linke, Dennis	Div. Systematic Proteome Research & Bioanalytics, Institute for Experimental Medicine, Kiel University, Germany	Combining 2D-LC-MS and Gelfree-LC-MS enhances both proteome coverage and the identification of short open reading frame encoded peptides
Linscheid, Michael	Humboldt-Universität zu Berlin	Collision Specific Fragmentation of Oligonucleotides in Tandem Mass Spectrometry Experiments Metal labelling of tri-functional Capture Compounds (CCs) to detect protein targets of small molecules
Linscheid, Michael W.	Humboldt-Universität zu Berlin, Institut für Chemie, Deutschland	A new internal standard approach for laser ablation ICP-MS of polyacrylamide gels Mass Spectrometry Imaging as Tool for the Analysis of MRI Contrast Agents in Biological Tissues Modifikation von Papiersubstraten mit hydrophoben Barrieren zur Erhöhung der Empfindlichkeit und Reproduzierbarkeit in der papierbasierten Massenspektrometrie
Lippert, Wayne	II physikalisches Insitut, Justus-Liebig-Universität Gießen, Deutschland	Tandem Mass Spectrometry with a (Ultra-)High Resolving Time-of-Flight Mass Spectrometer
Liu, Fan	Universiteit Utrecht, The Netherlands	Optimization of crosslinked peptide analysis on an Orbitrap Fusion Lumos mass spectrometer
Lockhauserbäumer, Julia	Heinrich-Pette-Institute Leibniz Institute for Experimental Virology, Deutschland	Studying viral capsid glycan interaction with native MS
Löhmannsröben, Hans-Gerd	University of Potsdam, Germany	IR-MALDI Ion Mobility Spectrometry: Low and High Field Mobilities of Peptide Ions at Intermediate Pressure
Lopez, Javier	Bruker Espanola S.A., Madrid, Spanien	Parts-per-trillion level high-throughput quantitation of glyphosate, aminomethylphosponic acid (AMPA) and glufosinate in water samples by LC-MS/MS
Lopez-Hilfiker, Felipe	TOFWERK, Schweiz; Paul Scherrer Institute (PSI), Villigen, Switzerland	Characterization of a New Extractive Electrospray Ionization (EESI) Source for Online Particle Analysis and its Application to Atmospheric Aerosol
Lorenz, Jana	1Department of Pharmaceutical Chemistry and Bioanalytics, Institute of Pharmacy, Martin-Luther University Halle-Wittenberg, Halle (Saale), Germany	Mass Spectrometry-Based Interaction Studies of the N-Terminus of the Formate Channel FocA from Escherichia coli Vortragend
Lorenz, Yvonne	Universität Bonn, Deutschland	ETD experiments on self-assembled asymmetric supramolecular squares Vortragend
Loroch, Stefan	Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund, Germany	Excellent sensitivity through excellent recovery – ERLIC for absolute quantification of low abundant protein phosphorylation events in cancer patient tissue Vortragend

Autor(en)	Organisation(en)	Titel des Beitrags
		Temporal quantitative phosphoproteomics of ADP stimulation reveals novel central nodes in platelet activation and inhibition
Lotz, Florian	Justus-Liebig-Universität Gießen, Deutschland	Development of an autarkic desorption electrospray ionization source for in-field DESI-MS applications Vortragend
Lubeck, Markus	Bruker Daltonik GmbH, Deutschland	Investigation of Q-TOF instruments advantages for label-free proteome analysis
Luckau, Luise	Physikalisch-Technische-Bundesanstalt, Deutschland	Precise quantification of HIV proteins by isotope dilution mass spectrometry (ID-MS) for applications in HIV diagnostics Vortragend
Luetjohann, Jens	GALAB Laboratories GmbH, Deutschland	Differentiation of organic and conventional farming of tomatoes by non-targeted metabolomic profiling using travelling-wave ion mobility high resolution mass spectrometry Vortragend
Luginbühl, Marc	Institute of Forensic Medicine, University of Bern	N-Acetyltaurine as a novel urinary ethanol marker in a drinking study Vortragend
Lukasheva, Elena	Universität St. Petersburg, Lehrstuhl Biochemie, Russia	Probing plant Maillard reaction by mass spectrometry in model peptide systems
Luo, Ruoji	Max-Planck-Institut für Kohlenforschung, Deutschland	Supercritical fluid extraction as a soil remediation method for removal of crude oil related contaminations, analyzed by FT Orbitrap MS Vortragend
Luo, Xian	Department of Chemistry, University of Alberta, Edmonton, Canada	Enabling High-Confidence Human Endogenous Metabolite Identification via High-Resolution MS/MS Retention-Time Library
Lupu, Loredana	Steinbeis Center for Biopolymer Analysis and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany; Proteome Center, Institute of Immunology, University of Rostock, Rostock, Germany	Innovative analytical methodologies for the development of new antitubercular agents
Lützen, Elias	Westfählische Wilhelms-Universität Münster	Molecular laser ablation-mass spectrometry for rapid identification of synthetic cannabinoids Vortragend
Maeser, Stefan	Steinbeis Center for Biopolymer Analysis and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany	Innovative analytical methodologies for the development of new antitubercular agents
Mairinger, Teresa	BOKU Wien, Österreich	Standardised Collision Cross Section Measurements by Single Static Drift Field Ion Mobility Instrument in an Interlaboratory Study
Makowski, Marcus R.	Charité, Berlin	Mass Spectrometry Imaging as Tool for the Analysis of MRI Contrast Agents in Biological Tissues
Mallagaray, Alvaro	Institute of Chemistry, University of Lübeck, Lübeck, Germany	Native mass spectrometry analysis of norovirus - glycan mimetics interaction
Mannaa, Atef	Mass Spectrometric Proteomics, Department of Clinical Chemistry, University Medical Center Hamburg-Eppendorf, Hamburg, Germany.	Sampling of tissues with the picosecond-infrared-laser ablation for Redox Proteomics Vortragend
Manns, Annika	Leibniz Institut für Molekulare Pharmakologie, Deutschland	Analysis of serine-phosphorylation dependent protein-protein interactions of the T cell adaptor protein ADAP Vortragend
Marcillo, Andrea	University of Leipzig, Germany	Methodological aspects of mass spectrometric detection for profiling ambient VOCs with thermodesorption-GCMS Vortragend The performance of mobile GC-MS for field sampling of body odours from common marmosets (Callithrix jacchus)
Marella, Chakravarthy	Research Center Borstel, Division of Bioanalytical Chemistry, Parkallee 1-40, D-23845 Borstel, Germany.	Lipidomes of human lung tissues show distinct lipid metabolic alterations for lung cancer and pulmonary emphysema
Marianski, Mateusz	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland	Glycan Fingerprinting using Cold-Ion Infrared Spectroscopy
Marshall, Peter	Departments of Platform Technology & Science, GlaxoSmithKline, Stevenage, UK	Ultra High Throughput Drug Discovery Screening by MALDI-TOF Mass Spectrometry
Martin, Diego	Bruker Espanola S.A., Madrid, Spanien	Parts-per-trillion level high-throughput quantitation of glyphosate, aminomethylphosponic acid (AMPA) and glufosinate in water samples by LC-MS/MS

Autor(en)	Organisation(en)	Titel des Beitrags
Massolini, Gabriella	Department of Drug Sciences, University of Pavia, Pavia, Italy	Innovative analytical methodologies for the development of new antitubercular agents
Matamoros, Manuel	Estación Experimental de Aula Dei, Consejo Superior de Investigaciones Científicas (CSIC), Department of Plant Nutrition	Age-related formation of advanced glycation end products (AGEs) in root nodules of common beans (Phaseolus vulgaris)
Matsubara, Shizue	IBG-2 Pflanzenwissenschaften, Forschungszentrum Jülich, Deutschland	Quantitative turnover analysis of chlorophylls, carotenoids and tocopherol in green leaves by LC-MS and FTICR-MS
Mattheij, Nadine J.	Department of Biochemistry, Cardiovascular Research Institute Maastricht, Maastricht University, The Netherlands;	Temporal quantitative phosphoproteomics of ADP stimulation reveals novel central nodes in platelet activation and inhibition
Mävers, Stephan	Bruker Daltonik GmbH, Deutschland	Boosting compound identification confidence in Metabolomics by exploiting all available Q-TOF high resolution accurate mass spectral information.
May, Jody	Vanderbilt University, USA	Standardised Collision Cross Section Measurements by Single Static Drift Field Ion Mobility Instrument in an Interlaboratory Study
Mazzone, Massimiliano	Laboratory of Molecular Oncology and Angiogenesis, Vesalius Research Center, Leuven, Belgium	Excellent sensitivity through excellent recovery – ERLIC for absolute quantification of low abundant protein phosphorylation events in cancer patient tissue
McGregor, Laura	Markes International, Gwaun Elai Medi-Science Campus, Llantrisant, RCT, Wales, United Kingdom	FAST MULTIPLEXING OF IONISATION ENERGY FOR PERFORMANCE IMPROVEMENTS IN GC-TOF MS
McLean, John	Vanderbilt University, USA	Standardised Collision Cross Section Measurements by Single Static Drift Field Ion Mobility Instrument in an Interlaboratory Study
McLean, Lynn	Centre for Proteome Research, Institute of Integrative Biology, University of Liverpool, Liverpool, UK	IMS-DIA-MS Characterisation and IMS-MRM QconCAT Quantitation of the Lipidome and Apolipoprotein Complements of Obesity and Diabetes Cohorts
Meckenstock, Rainer U.	Bio-film Center Universität Duisburg-Essen	Metabolite analysis of the phenanthrene degrading, sulfate reducing bacterial enrichment culture (TRIP) using GC-MS
Medvedev, Sergei	Department of Plant Physiology and Biochemistry, St. Petersburg State University, Russia	Profiles of glycated amino acid adducts in the protein hydrolyzates of pea (Pisum sativum) seeds subjected to accelerated ageing Simulated microgravity triggers transient enhancement of protein glycation and oxidation in germinating Brassica napus seeds
Mehmood, Tahir	Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry, Germany	Profiles of glycated amino acid adducts in the protein hydrolyzates of pea (Pisum sativum) seeds subjected to accelerated ageing
Meijers, Rob	European Molecular Biology Laboratory (EMBL), Hamburg, Germany	Structural characterization of protein-lipid complexes involved in clathrin-mediated endocytosis
Meiler, Jens	Vanderbilt University, Nashville, Tennessee, USA	Cross-Linking and Mass Spectrometry Shed New Light on the bMunc13-2/Calmodulin Interaction
Meinhardt, Ute	Friedrich-Alexander-University Erlangen-Nürnberg, Germany	Reactivity and stability check of even vs. odd electron (quasi)-molecular ions derived from triangulenium type derivatives
Melzig, Matthias F.	Freie Universität Berlin, Institute of Pharmacy, Pharmaceutical Biology	UPLC-ESI-QTOF-MS based chemical profiling of Actaea racemosa L. (black cohosh) rhizomes to investigate differences in cultivation, wild harvest, and genotypes
Memboeuf, Antony	UMR CNRS 6521, Université de Bretagne Occidentale, 6 Av.Le Gorgeu, 29200 Brest, France	COPPER-CATALYSED CLICK REACTION PERFORMED IN THE GAS PHASE: A COMBINED MASS SPECTROMETRIC AND DFT MECHANISTIC STUDY
Menezes, Riya Christina	Max Planck Institute for Chemical Ecology, Jena, Germany	Application of high-throughput MS screening to disentangle the bacterial metabolome Vortragend
Mercanoglu, Baris	University Medical Center Hamburg Eppendorf, Deutschland	Mass spectrometric characterization of aberrant O-glycosylation in COSMC deficient mouse pancreas tissue
Meyer, Bernd	Uni Hamburg, Deutschland	Analysis of human Glycoproteins with different LC-MS/MS and NMR techniques
Meyer, Nele	University of Bonn	Historical charcoal additions potentially improve stability of soil organic carbon

Autor(en)	Organisation(en)	Titel des Beitrags
Meyer, Stefanie	Friedrich Schiller University Jena, Deutschland	Effect of ecosystem type and fire on chemistry of WEOM as measured by LDI-TOF-MS and NMR
Meyer, Sven W.	Bruker Daltonik GmbH, Deutschland	High resolution trapped ion mobility mass spectrometry analysis of isomeric compounds
Michaelis, Simon	caprotec bioanalytics GmbH	Metal labelling of tri-functional Capture Compounds (CCs) to detect protein targets of small molecules
Michalski, Annette	Bruker Daltonik GmbH, Deutschland	Investigation of Q-TOF instruments advantages for label-free proteome analysis
Michalzik, Beate	Friedrich Schiller University Jena, Deutschland	Effect of ecosystem type and fire on chemistry of WEOM as measured by LDI-TOF-MS and NMR
Milentyev, Alexander	MPI-CBG, Dresden, Deutschland	Polyamine modifications in biosilica-associated proteome Vortragend
Milkovska-Stamenova, Sanja	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig; Center for Biotechnology and Biomedicine, Universität Leipzig	Protein carbonylation in raw milk and differently processed milk products Vortragend
Miller, Dwayne	Max Planck Institute for the Structure and Dynamics of Matter	Application of laser ablation for tissue metabolomics Lipidomics of Pig Brain Using the PIRL-DIVE Homogenisation Technique
Miller, Janet	Fort Collins Science Center, US Geological Survey, Fort Collins, USA	Investigating the zinc distribution in the mayfly N. triangulifer using elemental bioimaging by LA-ICP-MS
Miller, R. J. Dwayne	Max Planck Institut für Struktur und Dynamik der Materie, Hamburg, Deutschland; Department of Chemistry and Physics, University of Toronto, Toronto, Canada; Max Planck Institute for the Structure and Dynamics of Matter, Atomically Resolved Dynamics Division, Luruper Chaussee 149, 22761 Hamburg, Germany.	Development of Sub-Cellular Mass Spectrometry Imaging by Impulsive IR Laser Ablation Optimized Biomolecular Extraction Using Desorption by Impulsive Vibrational Excitation: Applications to Embryonic Cell Differentiation Sampling of tissues with the picosecond-infrared-laser ablation for Redox Proteomics
Milrud, Svetlana	Department of Plant Physiology and Biochemistry, St. Petersburg State University, Russia; Department of Biochemistry, St. Petersburg State University, Russia	Age-related glycation hotspots in plant proteome
Minameyer, Martin B.	Friedrich-Alexander-University Erlangen-Nürnberg, Germany	Formation and structure elucidation of $[M_2$ and $Ag]^+$ ions with M = [6]helicene, [7]helicene and coronene Formate attachment to ZnPorphyrin- and ZnPhthalocyanine-Oligomers: Binding, Fragmentation, Affinity Vortragend
Mindukshev, Igor	Sechenov Institute of Evolutionary Physiology and Biochemistry, Russian Academy of Sciences, Saint Petersburg, Russia;	Temporal quantitative phosphoproteomics of ADP stimulation reveals novel central nodes in platelet activation and inhibition
Mischnick, Petra	Technische Universität Braunschweig, Deutschland	Precise quantification of HIV proteins by isotope dilution mass spectrometry (ID-MS) for applications in HIV diagnostics
Miske, Ramona	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	The role of mass spectrometry in the identification of autoantigens as targets in neurological autoimmune diseases
Mitrofanov, Elena	Christian-Albrechts-Universität, Deutschland	Wellenlängenabhängige Photofragmentierung von fluoreszierenden Farbstoffen in einem FT-ICR Massenspektrometer Vortragend
Mnatsakanyan, Ruzanna	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig; Center for Biotechnology and Biomedicine, Universität Leipzig	Protein carbonylation in raw milk and differently processed milk products

Autor(en)	Organisation(en)	Titel des Beitrags
Möbius, Wiebke	Department of Neurogenetics, Max-Planck-Institute of Experimental Medicine, 37075 Göttingen, Germany; Center for Nanoscale Microscopy and Molecular Physiology of the Brain, 37075 Göttingen, Germany	Partial Immunoblotting of 2D-Gels: A Novel Method to Identify Post-Translationally Modified Proteins Exemplified for the Myelin Acetylome
Mock, Hans-Peter	IPK-Gatersleben, Deutschland	Characterization of plastidal redox-responses during cold stress acclimation
Moise, Adrian	Department of Chemistry, University of Konstanz, Konstanz, Germany	CHARACTERIZATION OF CARBOHYDRATE BINDING SITES IN GALECTINS BY PROTEOLYTIC AFFINITY - MASS SPECTROMETRY
Mokhtar, Mohamed	Christian-Albrechts-Universität zu Kiel, Deutschland	Improving the sequence coverage in top-down MS/MS of proteins
Möller, Manfred	Uniklinik der RWTH Aachen, Deutschland	The performance of mobile GC-MS for field sampling of body odours from common marmosets (Callithrix jacchus)
Möller, Stephanie	Biomaterials Department, INNOVENT e.V., Jena, Germany	Comparative analysis of the effects of sulfated hyaluronic acid and dexamethasone on osteoblast differentiation by nanoLC-MS and random forest modeling.
Mordehai, Alex	Agilent Technologies, Santa Clara, USA	Standardised Collision Cross Section Measurements by Single Static Drift Field Ion Mobility Instrument in an Interlaboratory Study
Morgner, Nina	Johann Wolfgang Goethe-Universität, Deutschland; University of Frankfurt, Deutschland; Institut für Physikalische und Theoretische Chemie, Goethe-Universität Frankfurt	Analyzing macromolecular complexes: subunit interactions of the F1F0 ATP synthase and conformational changes of the heterodimeric ABC transport complex TmrAB Applications of non-covalently bound membrane proteins in nanodiscs using LILBID-MS Characterizing the LILBID ionization method: energy transfer and dissociation From Salty to Salt-free: Monitoring the Salt-dependent Dissoziation of the Membrane Protein Complex GCD in a Single Experiment Monitoring and correlating of protein charge states with respect to amino acid modification and buffer conditions Steps towards a more native analysis of Aß42 using LILBID mass spectrometry
Mormann, Michael	Institut für Hygiene, Universität Münster, Deutschland	Identification of an unusual N-glycan detected in a tryptic glycopeptide derived from intergrin α7 expressed in Drosophila S2 cells Towards qMALDI-MSI : MS imaging of phospholipids in mouse cerebellum followed by semi-quantitative nano-HPLC-ESI-MS of extracts from laser micro-dissected brain regions
Morrice, Nick	SCIEX, UK	Accelerating Data Independent Acquisition with Microflow Chromatography
Mucek, Katharina	Bioanalytical Mass Spectrometry, Max Planck Institute for Biophysical Chemistry, Göttingen, Germany	Analysis of 1,2,3,4-diepoxybutane induced DNA-histone cross-links by mass spectrometry Vortragend
Mucha, Eike	Freie Universität Berlin, Deutschland; Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland	Glycan Fingerprinting using Cold-Ion Infrared Spectroscopy
Mueller, Jennifer-Christin	Institute of Inorganic and Analytical Chemistry, University of Muenster, Corrensstr. 28/30, 48149 Muenster, Germany	Analysis of Liquid Crystal Display Sealants using Spatially Resolved Mass Spectrometric Methods Vortragend
Mueller, Max A.	Justus Liebig University Giessen, Germany	Implementation of a High Repetition-Rate Laser System in an AP-SMALDI MSI System for Enhanced Measurement Speed
Mülbaier, Marcel	Cellzome GmbH, Heidelberg	Analysis of drug-induced effects on proteostasis in cell lines and non-dividing primary cells by quantitative mass spectrometry
Müller, Julia	Pathology of the University Hospital of Lübeck and the Research Center Borstel, Clinical and Experimental Pathology, 23538 Lübeck and 23845 Borstel, Germany.	Lipidomes of human lung tissues show distinct lipid metabolic alterations for lung cancer and pulmonary emphysema
Müller, Katrin	Cellzome GmbH, Heidelberg	Analysis of drug-induced effects on proteostasis in cell lines and non-dividing primary cells by quantitative mass spectrometry

Autor(en)	Organisation(en)	Titel des Beitrags
Müller, Mathias	Thermo Fisher Scientific, Bremen, Germany	Optimization of crosslinked peptide analysis on an Orbitrap Fusion Lumos mass spectrometer Vortragend
Müller, Miriam J.	Universität des Saarlandes, Saarbrücken, Deutschland; Saarland University, Deutschland	Vitamin D3 epimers: analytical nuisance or clinical opportunity? Direct aqueous measurement of 25-hydroxyvitamin D in cellular environments by LC-MS/MS using the novel chemical derivatization reagent MDBP Vortragend
Müller, Volker	Johann Wolfgang Goethe-Universität, Deutschland	Analyzing macromolecular complexes: subunit interactions of the F1F0 ATP synthase and conformational changes of the heterodimeric ABC transport complex TmrAB
Mung, Dorothea	Department of Chemistry, University of Alberta, Edmonton, Canada	Enabling High-Confidence Human Endogenous Metabolite Identification via High-Resolution MS/MS Retention-Time Library
Muñoz-Fontela, Cesar	Heinrich-Pette-Institut, Hamburg, Deutschland	Analyzing self-assembly of Ebola virus nucleoprotein with native mass spectrometry
Münster-Müller, Sascha	Bundeskriminalamt Wiesbaden	Molecular laser ablation-mass spectrometry for rapid identification of synthetic cannabinoids
Muskat, Tassilo	Christian-Albrechts-Universität, Deutschland	Wellenlängenabhängige Photofragmentierung von fluoreszierenden Farbstoffen in einem FT-ICR Massenspektrometer
Näthe, Kerstin	Friedrich Schiller University Jena, Deutschland	Effect of ecosystem type and fire on chemistry of WEOM as measured by LDI-TOF-MS and NMR
Neese, Stephan	Justus-Liebig-Univeristät Gießen, Deutschland	Real-time food authentication with a miniature mass spectrometer
Neubauer, Lisa	Institute of Plant Biology and Biotechnology, University of Münster, Germany	Localization of Ergot Alkaloids in Sclerotia of Claviceps purpurea by MALDI-MS Imaging
Neugebauer, Thomas	Friedrich-Alexander-University Erlangen-Nürnberg, Deutschland	Formation and dissociation behavior of multiply charged salt-like cluster ions (sodium formate) Vortragend
Neumann, Anika	Joint Mass Spectrometry Centre / Chair of Analytical Chemistry, University of Rostock, 18059 Rostock, Germany	Evolved gas analysis ultra high resolution mass spectrometry - Insights into heavy petroleum fractions and combustion aerosol Thermal and laser desorption atmospheric pressure photo ionisation ultra high resolution mass spectrometry – Concept and application towards complex samples Vortragend
Neumann, Heinz	Free Floater (Junior) Research Group Applied Synthetic Biology, Georg-August University Göttingen, Institute for Microbiology and Genetics, 37077 Göttingen, Germany	Partial Immunoblotting of 2D-Gels: A Novel Method to Identify Post-Translationally Modified Proteins Exemplified for the Myelin Acetylome
Neupärtl, Moritz	Goethe-Universität-Frankfurt	ArgC-like digestion: complementary or alternative to tryptic digestion?
Neuweger, Heiko	Bruker Daltonik GmbH, Deutschland	Boosting compound identification confidence in Metabolomics by exploiting all available Q-TOF high resolution accurate mass spectral information. Metabolomics to study the “war” between plants and insects - Systemic defense induction and post-ingestive rearrangement of plant toxins in insects.
Neuwohner, Andrea	IBG-2 Pflanzenwissenschaften, Forschungszentrum Jülich, Deutschland	Quantitative turnover analysis of chlorophylls, carotenoids and tocopherol in green leaves by LC-MS and FTICR-MS
Nguyen, Minh	ISAS, Deutschland	Simple, scalable and sensitive tip-based enrichment of N-terminal peptides for profiling of protease substrates
Ni, Zhixu	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig; Center for Biotechnology and Biomedicine, Universität Leipzig, Germany	oxLipidomics data integration for systems medicine view on metabolic diseases
NicDaeid, Niamh	University of Dundee, CAHID, School of Science and Engineering, Dundee, DD15EH, Scotland	Development and implementation of new analytical methods and databases for the detection of additives in fuels and fire debris.
Niehoff, Ann-Christin	University of Münster, Institute of Inorganic and Analytical Chemistry, Münster, Germany	Bioimaging of photosensitizers in human brain tumors after fluorescence-guided resection
Nikolaev, Eugene N.	Institute for Energy Problems of Chemical Physics, Russian	MALDI FT-ICR Imaging: Double the Performance or Double the Samples using Quadrupolar Detection 2ω-FT-ICR Mass Spectrometry with Quadrupolar Detection

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	Academy of Sciences, Moscow, Russia	
O'Hair, Richard	University of Melbourne, Australia	Coinage-Metal Ate Complexes – An ESI-MS Study
Oefner, Peter J.	University of Regensburg, Institute of Functional Genomics, Regensburg, Deutschland	A step forward in GC-HRAM-MS based metabolomics - A novel atmospheric pressure GC-APCI Source increases quantitative and qualitative performance
Opuni, Kwabena F.M.	Proteome Center Rostock, Deutschland	Intact Transition Epitope Mapping - A mass spectrometric method for accurate, facile, and rapid identification of specific antibody-peptide reactivities
Oster, M.	2Joint Mass Spectrometry Centre Helmholtz-Zentrum München, Comprehensive Molecular Analytics (CMA), Neuherberg, Germany	Multiple analysis of individual airborne aerosol particles by laser mass spectrometry: Detection of polyaromatic hydrocarbons from the particle-surface and particle-core
Othman, Alaa	University of Lübeck, Germany	LC/MS²-standards library using high-resolution accurate mass (HRAM) platform for metabolomics research
O'Hair, Richard A. J.	The University of Melbourne, Australia	Adventures with Mass Spectrometers: From Designing New Catalysts to Developing a Non-Targeted Drug Metabolite Identification Procedure. Vortragend
Pagel, Kevin	Freie Universität Berlin, Deutschland; Fritz-Haber-Institut Berlin, Deutschland; Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin	Following the Unfolding and Dissociation of Calmodulin/Munc13 Complexes by Ion Mobility-Mass Spectrometry Glycan Fingerprinting using Cold-Ion Infrared Spectroscopy Vortragend Investigation of Dimeric and Hexameric Halogen-Bonded Supramolecular Capsules by ESI-MS and IM-MS The Amyloid Formation Mechanism of Human IAPP: An Infrared Spectroscopy Approach
Papan, Cyrus	SCIEX GmbH, Darmstadt, GERMANY	SelexION® DMS-based detergent interference removal for shotgun-lipidomics analyses Vortragend
Parchomyk, Tobias	Georg-August-Universität Göttingen, Deutschland	Direct Observation and Reactivity Studies of Organoferrates by Electrospray Ionization Mass Spectrometry Vortragend
Passig, Johannes	Universität Rostock, Deutschland; Joint Mass Spectrometry Centre University of Rostock, Chair of Analytical Chemistry, Rostock, Germany	Direct resonance-enhanced multi-photon ionisation (REMPI) of complex liquid samples under vacuum conditions Multiple analysis of individual airborne aerosol particles by laser mass spectrometry: Detection of polyaromatic hydrocarbons from the particle-surface and particle-core Vortragend
Paudel, Gagan	Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry (Halle/Saale); Faculty of Chemistry and Mineralogy, Universität Leipzig	Age-related glycation hotspots in plant proteome
Paudyal, Bhesh Raj	Department of Cellular Microbiology, Research Center Borstel, Parkallee 22, Borstel, Germany	Software platform to improve the quality control of Lipid mediator quantification
Peetz, Oliver	University of Frankfurt, Deutschland	Applications of non-covalently bound membrane proteins in nanodiscs using LILBID-MS Vortragend
Peng, Bing	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Germany	A new bridge between targeted and non-targeted LC-MS/MS lipidomics Vortragend
Penkert, Martin	Leibniz-Institut für molekulare Pharmakologie (FMP), Deutschland; Humboldt-Universität zu Berlin	Neutral loss-triggered EThcD mass spectrometry identifies protein pyrophosphorylation in vivo Vortragend
Penner, Alexander	Justus-Liebig-Univeristät Gießen, Deutschland	Real-time food authentication with a miniature mass spectrometer
Perez, Cesar	Bruker Espanola S.A., Madrid, Spanien	Parts-per-trillion level high-throughput quantitation of glyphosate, aminomethylphosponic acid (AMPA) and glufosinate in water samples by LC-MS/MS
Persicke, Marcus	Bielefeld University, Bielefeld, Deutschland	Boosting compound identification confidence in Metabolomics by exploiting all available Q-TOF high resolution accurate mass spectral information.
Peters, Thomas	Institute of Chemistry, University of Lübeck, Lübeck, Germany	Native mass spectrometry analysis of norovirus - glycan mimetics interaction

Autor(en)	Organisation(en)	Titel des Beitrags
Pietschke, Cleo	Zoologisches Institut, Uni Kiel	Identification and characterization of N-acyl homoserine lactones by mass spectrometry
Pikhtelev, Alexander	Institute of Energy Problems of Chemical Physics, Russian Academy of Sciences, Russia	Tandem Mass Spectrometry with a (Ultra-)High Resolving Time-of-Flight Mass Spectrometer
Piotrowski, Christine	Martin-Luther-Universität Halle-Wittenberg, Deutschland	Cross-Linking and Mass Spectrometry Shed New Light on the bMunc13-2/Calmodulin Interaction Vortragend
Planitz, Peter	Agilent Technologies, Waldbronn, Germany	Elemental Bioimaging by LA-ICP-QQQ-MS for the Investigation of Wilson´s Disease
Plaß, Wolfgang R.	II physikalisches Insitut, Justus-Liebig-Universität Gießen, Deutschland; GSI Darmstadt, Deutschland	Tandem Mass Spectrometry with a (Ultra-)High Resolving Time-of-Flight Mass Spectrometer
Poeckel, Daniel	Cellzome GmbH, Heidelberg	Analysis of drug-induced effects on proteostasis in cell lines and non-dividing primary cells by quantitative mass spectrometry
Pogan, Ronja	Heinrich-Pette-Institute Leibniz Institute for Experimental Virology, Deutschland	Studying viral capsid glycan interaction with native MS Vortragend
Pohlentz, Gottfried	Institut für Hygiene, Universität Münster, Deutschland	Identification of an unusual N-glycan detected in a tryptic glycopeptide derived from intergrin α7 expressed in Drosophila S2 cells Vortragend
Popkova, Yulia	Leipzig University, Faculty of Medicine, Institute for Medical Physics and Biophysics, Germany	Selective triacylglycerol suppression in complex lipid mixtures by CsCl addition Vortragend
Pospilova, Veronika	Paul Scherrer Institute (PSI), Villigen, Switzerland	Characterization of a New Extractive Electrospray Ionization (EESI) Source for Online Particle Analysis and its Application to Atmospheric Aerosol
Potthoff, Alexander	Institute for Hygiene, University of Münster, Robert-Koch-Str. 41, 48149 Münster, Germany	The internal energy in a MALDI plume probed with thermometer molecules: Effects of laser excitation wavelength and laser fluence Vortragend
Pötz, Oliver	Natural and Medical Sciences Institute at the University of Tübingen, Tübingen, Germany;	Temporal quantitative phosphoproteomics of ADP stimulation reveals novel central nodes in platelet activation and inhibition
Poulsen, Nicole	B-CUBE Center for Molecular Bioengineering, Dresden, Deutschland	Polyamine modifications in biosilica-associated proteome
Prasse, Daniela	Institute for General Microbiology, Kiel University, Germany	Combining 2D-LC-MS and Gelfree-LC-MS enhances both proteome coverage and the identification of short open reading frame encoded peptides
Probst, Christian	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	The role of mass spectrometry in the identification of autoantigens as targets in neurological autoimmune diseases
Przybylski, Michael	Steinbeis Centre Biopolymer Analysis & Biomedical Mass Spectrometry, Rüsselsheim, Germany	CHARACTERIZATION OF CARBOHYDRATE BINDING SITES IN GALECTINS BY PROTEOLYTIC AFFINITY - MASS SPECTROMETRY Innovative analytical methodologies for the development of new antitubercular agents
Pütz, Michael	Bundeskriminalamt Wiesbaden	Molecular laser ablation-mass spectrometry for rapid identification of synthetic cannabinoids
Quack, Thomas	Justus-Liebig-Universität Gießen, Institut für Parasitologie	AP-SMALDI MSI of metabolites and lipids in Schistosoma mansoni parasites
Rabe, Klaus F.	LungenClinic Großhansdorf, Wöhrendamm 80, 22927 Großhansdorf.; Airway Research Center North, German Center for Lung Research, Wöhrendamm 80, 22927 Großhansdorf, Germany	Lipidomes of human lung tissues show distinct lipid metabolic alterations for lung cancer and pulmonary emphysema
Raja, Erum	Thermo Fisher Scientific, Rockford, IL, USA	Optimization of crosslinked peptide analysis on an Orbitrap Fusion Lumos mass spectrometer
Raupers, Björn	Universität Kiel, Deutschland	Untersuchung von Limonen-Clustern im LTP-Twin-Trap Massenspektrometer Vortragend

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Rehkamp, Anne	Martin-Luther-University Halle-Wittenberg, Institute of Pharmacy, Department of Pharmaceutical Chemistry and Bioanalytics, Germany	Structural Insights into Retinal Guanylyl Cyclase/GCAP-2 Interaction by Cross-linking and Mass Spectrometry Vortragend
Reinert, Thorben	Christian-Albrechts-Universität zu Kiel, Deutschland	REMPI-Spektroskopie von nicht-kovalenten Anisol-Clustern Vortragend
Renné, Thomas	University Medical Center Hamburg Eppendorf, Deutschland	Proteome-wide detection of proteolysis in blood plasma by the SDS-PAGE-migration profile
Rennie, Emma	Agilent Technologies, Santa Clara, USA	Standardised Collision Cross Section Measurements by Single Static Drift Field Ion Mobility Instrument in an Interlaboratory Study
Reuter, Jörn Hendrik	Research and Development, Beiersdorf AG, Hamburg	Proteomic investigation of skin cell layers by tissue ablation using picosecond infrared laser (PIRL)
Richardson, Keith	Waters Corporation, Wilmslow, United Kingdom	Lipidomics Quantitation Using a Novel Scanning Quadrupole DIA Method Quantitation of Proteomics Samples Using a Novel Scanning Quadrupole DIA Method
Riebe, Daniel	University of Potsdam, Germany	IR-MALDI Ion Mobility Spectrometry: Low and High Field Mobilities of Peptide Ions at Intermediate Pressure
Riedel, Jens	Bundesanstalt für Materialforschung- und prüfung, Deutschland	Collision Specific Fragmentation of Oligonucleotides in Tandem Mass Spectrometry Experiments Improving the performance of the airborne laser-spark ion source for the detection of volatile organic compounds under ambient conditions Modifikation von Papiersubstraten mit hydrophoben Barrieren zur Erhöhung der Empfindlichkeit und Reproduzierbarkeit in der papierbasierten Massenspektrometrie
Riemer, Thomas	University of Leipzig, Medical Faculty, Institute of Medical Physics and Biophysics	Differentiation and relative quantification of chondroitin sulfate isomers by ion mobility spectrometry-mass spectrometry and pulsed-field gradient NMR
Rinaldi, Francesca	Department of Drug Sciences, University of Pavia, Pavia, Italy	Innovative analytical methodologies for the development of new antitubercular agents Vortragend
Rissanen, Kari	Department of Chemistry, NanoScience Center, University of Jyvaskyla, Finnland	Investigation of Dimeric and Hexameric Halogen-Bonded Supramolecular Capsules by ESI-MS and IM-MS
Robertson, Wesley D.	Max Planck Institut für Struktur und Dynamik der Materie, Hamburg, Deutschland	Development of Sub-Cellular Mass Spectrometry Imaging by Impulsive IR Laser Ablation Optimized Biomolecular Extraction Using Desorption by Impulsive Vibrational Excitation: Applications to Embryonic Cell Differentiation
Röcken, Christoph	Institute of Pathology, Christian-Albrechts-Universität, Kiel, Germany	Identification and classification of amyloidosis by matrix-assisted laser desorption/ionization mass spectrometry imaging
Roeck, Walter	Bruker BioSpin AG, Fällanden, Switzerland	2ω-FT-ICR Mass Spectrometry with Quadrupolar Detection
Rohn, Sascha	Universität Hamburg, Deutschland; Universität Hamburg, Grindelallee 117, Hamburg	Discrimination of apple and potato cultivars by non-targeted metabolomic fingerprinting via UPLC-IMS-QToF analysis Quality assessment of olive oil based on volatile compound fingerprinting using HRGC-IMS analysis
Rohner, Urs	TOFWERK, Switzerland	Determination of multi-element composition and mass of single nanoparticles in liquids and air Vortragend
Romanovskaya, Ekaterina	Department of Biochemistry, St. Petersburg State University, Russia	Profiles of glycated amino acid adducts in the protein hydrolyzates of pea (Pisum sativum) seeds subjected to accelerated ageing
Römpp, Andreas	Department of Food Analysis, University of Bayreuth, E.-C.-Baumann-Str. 20, 95326 Kulmbach, Bayreuth, Germany; Chair of Bioanalytical Sciences and Food Analysis, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth, Germany; Universität Bayreuth, Deutschland	Imaging metabolites in wheat stem base-Fusarium graminearum interactions using high-resolution atmospheric pressure scanning microprobe MALDI mass spectrometry imaging (SMALDI-MSI) imzML - Current status and future perspectives of the open standard for mass spectrometry imaging data Vortragend Multimodal imaging combining mass spectrometry and vibrational spectroscopy using a single tissue section and an integrated data processing workflow Overview of imzML-based software tools for MS imaging
Roth, Alexander	Hochschule Mannheim, Deutschland	Derivatization of low-volatile compounds in aqueous solution and analysis by HS-GC-IMS Vortragend
Rüger, Christopher Paul	University of Rostock, Rostock;	The Usage of Direct Inlet Probe in combination with High Resolution Mass Spectrometry for the Characterization of Heavy Petroleum

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	Joint Mass Spectrometry Centre / Chair of Analytical Chemistry, University of Rostock, 18059 Rostock, Germany	Products Thermal and laser desorption atmospheric pressure photo ionisation ultra high resolution mass spectrometry – Concept and application towards complex samples Evolved gas analysis ultra high resolution mass spectrometry - Insights into heavy petroleum fractions and combustion aerosol Vortragend
Rühl, Michael	Goethe Universität Frankfurt, Deutschland	CICCA-Tetrazole: An alternative matrix for the analysis of low molecular weight compounds by MALDI-MS Investigating on-plate digestion of proteins with regard to trypsin activity and oxidation Vortragend
Rurack, Knut	Bundesanstalt für Materialforschung und -prüfung	Modifikation von Papiersubstraten mit hydrophoben Barrieren zur Erhöhung der Empfindlichkeit und Reproduzierbarkeit in der papierbasierten Massenspektrometrie
Rutjens, Sofie	Laboratory of Toxicology, University of Ghent	N-Acetyltaurine as a novel urinary ethanol marker in a drinking study
Rychlik, Michael	Technische Universität Münschen, Lehrstuhl für Analytische Lebensmittelchemie	Validierung einer Stabilisotopenverdünnungsanalyse von Folaten in Lebensmitteln und Bestimmung des Folatgehaltes in Naturprodukten
Saluz, Hans Peter	Department Cell and Molecular Biology, Leibniz Institute for Natural Product Research and Infection Biology	Mapping metabolites from rough terrain: laser ablation electrospray ionization on non-flat samples
Sanchez-Carballo, Patricia	Division of Clinical Infectious Diseases, Research Center Borstel, Borstel, Germany; German Center for Infection Research, Clinical Tuberculosis Center, Borstel, Germany	LC-MS2 Method Development for Simultaneous Analysis of Antibiotics from Plasma of MDR-TB Patients
Satilmis, Ilker	Max-Planck-Institut für Kohlenforschung, Deutschland	Fenton based oxidation of crude oil in supercritical CO2 Vortragend
Sauerland, Volker	Bruker Daltonik GmbH, Germany	Ultra High Throughput Drug Discovery Screening by MALDI-TOF Mass Spectrometry
Savitski, Mikhail M.	Cellzome GmbH, Heidelberg; EMBL, Heidelberg	Analysis of drug-induced effects on proteostasis in cell lines and non-dividing primary cells by quantitative mass spectrometry
Sawers, Gary	2Department of Microbiology, Institute of Biology, Martin-Luther University Halle-Wittenberg, Halle (Saale), Germany	Mass Spectrometry-Based Interaction Studies of the N-Terminus of the Formate Channel FocA from Escherichia coli
Schachel, Tilo D.	Westfälische Wilhelms-Universität Münster, Deutschland	Differentiation and Identification of Explosives Formulations by Means of HPLC-MS Vortragend
Schade, Julian	Joint Mass Spectrometry Centre University of Rostock, Chair of Analytical Chemistry, Rostock, Germany	Multiple analysis of individual airborne aerosol particles by laser mass spectrometry: Detection of polyaromatic hydrocarbons from the particle-surface and particle-core
Schäfer, Frank	Federal Criminal Police Office, Forensic Institute, 65193 Wiesbaden, Germany	Development and implementation of new analytical methods and databases for the detection of additives in fuels and fire debris.
Schäfer, Mathias	Institute for Organic Chemistry, Department of Chemistry, University of Cologne; Universität zu Köln, Deutschland	An Integrated Workflow for Structural Proteomics Studies based on Cross-linking/Mass Spectrometry with an MS/MS Cleavable Cross-linker Synthesis of Isotope-Labeled Derivatives of the MS/MS-Cleavable Urea-Cross-Linker: Synthesis and Evaluation of Reactivity for Effective Protein Structure Analysis Dissociation behavior of a TEMPO-benzyl cross-linker for peptide structure analysis by free radical initiated peptide sequencing (FRIPS) in negative ESI-MS
Schäfer, Mathias	Institute of Organic Chemistry, University of Cologne, Greinstraße 4, 50939 Köln, Germany	Software platform to improve the quality control of Lipid mediator quantification
Schaible, Ulrich E.	Department of Cellular Microbiology, Research Center Borstel, Parkallee 22, Borstel, Germany	Software platform to improve the quality control of Lipid mediator quantification

Autor(en)	Organisation(en)	Titel des Beitrags
Schalley, Christoph A.	Freie Universität Berlin	Investigation of Dimeric and Hexameric Halogen-Bonded Supramolecular Capsules by ESI-MS and IM-MS
Scharf, Madeleine	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	The role of mass spectrometry in the identification of autoantigens as targets in neurological autoimmune diseases
Scharrenbroch, Lisa	Federal Criminal Police Office, Forensic Institute, 65193 Wiesbaden, Germany; University of Dundee, CAHID, School of Science and Engineering, Dundee, DD15EH, Scotland	Development and implementation of new analytical methods and databases for the detection of additives in fuels and fire debris. Vortragend
Schatz, Jürgen	Friedrich-Alexander-University Erlangen-Nürnberg, Germany	Reactivity and stability check of even vs. odd electron (quasi)-molecular ions derived from triangulenium type derivatives
Scheeren, Simon Gereon	Westfälische Wilhelms-Universität Münster, Deutschland	Automated electrochemistry/mass spectrometry for high-throughput analysis of xenobiotics Vortragend
Scheffler, Kai	Thermo Fisher Scientific, Deutschland	Evaluation of Optimal Conditions for Antibody Subunit Analysis on a Quadrupole-Orbitrap Mass Spectrometer Full Characterization of Antibodies Under Denaturing and Native Conditions on a Hybrid Quadrupole-Orbitrap MS Equipped With a Higher Mass Range
Scheidegger, Oliver	Hoffmann la Roche AG, Schweiz	Field ionization: an old but still useful method
Scheidenberger, Christoph	II physikalisches Insitut, Justus-Liebig-Universität Gießen, Deutschland; GSI Darmstadt, Deutschland	Tandem Mass Spectrometry with a (Ultra-)High Resolving Time-of-Flight Mass Spectrometer
Scheier, Rico	Universität Bayreuth, Deutschland	Multimodal imaging combining mass spectrometry and vibrational spectroscopy using a single tissue section and an integrated data processing workflow
Schelhaas, Mario	Institute of Molecular Virology & Institute of Medical Biochemistry Münster, WW University of Münster, Germany	Studying viral capsid glycan interaction with native MS
Schenk, Regina	Humboldt-Universität zu Berlin, Albrecht Daniel Thaer-Institute for Crop Science	UPLC-ESI-QTOF-MS based chemical profiling of Actaea racemosa L. (black cohosh) rhizomes to investigate differences in cultivation, wild harvest, and genotypes
Schiller, Jürgen	University of Leipzig, Medical Faculty, Institute of Medical Physics and Biophysics	Differentiation and relative quantification of chondroitin sulfate isomers by ion mobility spectrometry-mass spectrometry and pulsed-field gradient NMR Selective triacylglycerol suppression in complex lipid mixtures by CsCl addition
Schilyaev, Nikita	Universität St. Petersburg, Lehrstuhl Biochemie, Russia	Probing plant Maillard reaction by mass spectrometry in model peptide systems
Schlichting, Rita	Helmholtz-Centre for Environmental research (UFZ), Department of Cell Toxicology, Leipzig, Germany	Phthalate metabolites MEHP and MEOHP but not the phthalate DEHP itself bind and activate the PPARγ
Schlüter, Hartmut	University Medical Center Hamburg-Eppendorf, Deutschland	Comparison of Data-Independent Acquisition (DIA) and Data-Dependent Acquisition (DDA) for label-free Quantification Mass spectrometric characterization of aberrant O-glycosylation in COSMC deficient mouse pancreas tissue Application of laser ablation for tissue metabolomics Comparison of label free quantification methods for proteomics
Schlüter, Hartmut	University Medical Centre Hamburg-Eppendorf, Institute of Clinical Chemistry, Department for Mass Spectrometric Proteomics, Hamburg Germany; Universitätsklinikum Hamburg-Eppendorf, Germany; University Medical Center Hamburg Eppendorf, Deutschland; Mass Spectrometric Proteomics, Department of	Lipidomics of Pig Brain Using the PIRL-DIVE Homogenisation Technique Mass spectrometry evaluation of the Etanercept physicochemical properties Proteome-wide detection of proteolysis in blood plasma by the SDS-PAGE-migration profile Proteomic investigation of skin cell layers by tissue ablation using picosecond infrared laser (PIRL) Sampling of tissues with the picosecond-infrared-laser ablation for Redox Proteomics

Autor(en)	Organisation(en)	Titel des Beitrags
	Clinical Chemistry, University Medical Center Hamburg-Eppendorf, Hamburg, Germany.	
Schmid, Robin	Institute of Food Chemistry, University of Münster, Germany; Institute of Inorganic and Analytical Chemistry, University of Münster, Germany	Algorithms for the annotation of isotopes, fragments and adducts, applied to HPLC-HRMS metabolomics data for the discovery of novel compounds Vortragend
Schmidt, Carla	Interdisciplinary research center HALOmem, Martin Luther University Halle-Wittenberg, Kurt-Moses-Straße-3, 06120 Halle (Saale).	Development of a protein interaction networks in synaptic vesicles using cross-linking and mass spectrometry Ligand induced oligomerisation of proteins – insights from mass spectrometry Vortragend Fragmentation behavior of neuronal lipids by HCD-MS/MS
Schmidt, Charlie	PerkinElmer LAS (Germany) GmbH, Deutschland	Rapid On Site Analysis of BTX with Portable GC/MS
Schmidt, Heinar	Universität Bayreuth, Deutschland	Multimodal imaging combining mass spectrometry and vibrational spectroscopy using a single tissue section and an integrated data processing workflow
Schmidt, Johannes R.	Department for Molecular Systems Biology, Helmholtz Centre for Environmental Research – UFZ, Leipzig, Germany	Comparative analysis of the effects of sulfated hyaluronic acid and dexamethasone on osteoblast differentiation by nanoLC-MS and random forest modeling. Vortragend
Schmidt, Rico	Institute of Pharmacy, Martin-Luther Universität Halle-Wittenberg	Age-related glycation hotspots in plant proteome Simulated microgravity triggers transient enhancement of protein glycation and oxidation in germinating Brassica napus seeds
Schmidt, Travis	Fort Collins Science Center, US Geological Survey, Fort Collins, USA	Investigating the zinc distribution in the mayfly N. triangulifer using elemental bioimaging by LA-ICP-MS
Schmit, Pierre-Olivier	Bruker Daltonique Wissembourg, France; Bruker Daltonik GmbH, Deutschland	Applying a Proteoform profiling method for neurological disorder biomarker discovery operations Investigation of Q-TOF instruments advantages for label-free proteome analysis
Schmitt-Kopplin, Philippe	Helmholtz Zentrum München, Deutschland; Technische Universität München	Power-function Resolution Filter in Fourier Transform Mass Spectrometry
Schmitz, Ruth A.	Institute for General Microbiology, Kiel University, Germany	Combining 2D-LC-MS and Gelfree-LC-MS enhances both proteome coverage and the identification of short open reading frame encoded peptides
Schnapp, Andreas	Institute for Hygiene, Biomedical Mass Spectrometry, University of Münster, Germany; Institute for Hygiene, University of Münster, Robert-Koch-Str. 41, 48149 Münster, Germany	Elucidation of double bond positions in lipids by means of off-line ozonolysis followed by ultraviolet laser desorption ionization mass spectrometry Single-photon ionization of laser desorbed molecules in a fine-vacuum ion source
Schöllkopf, Wieland	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland	Glycan Fingerprinting using Cold-Ion Infrared Spectroscopy
Scholz, Verena	Research Center Borstel, Division of Bioanalytical Chemistry, Parkallee 1-40, D-23845 Borstel, Germany.	Lipidomes of human lung tissues show distinct lipid metabolic alterations for lung cancer and pulmonary emphysema
Schönborn, Stefan	Goethe-Universität Frankfurt am Main, Deutschland	Investigating on-plate digestion of proteins with regard to trypsin activity and oxidation
Schrader, Wolfgang	Max-Planck-Institut für Kohlenforschung, Deutschland	APPI-FAIMS-FTMS source and electrode optimization for the elucidation of structural features of crude oil constituents Characterization of Fast-Pyrolysis Bio-Oil Fenton based oxidation of crude oil in supercritical CO2 Metabolite analysis of the phenanthrene degrading, sulfate reducing bacterial enrichment culture (TRIP) using GC-MS Supercritical fluid extraction as a soil remediation method for removal of crude oil related contaminations, analyzed by FT Orbitrap MS Effect of temperature on crude oil fouling under inert and oxygenated conditions and subsequent analysis by HRMS

Autor(en)	Organisation(en)	Titel des Beitrags
		Electrospray Fourier Transform ion cyclotron resolution mass spectrometry: reactivity of polyaromantic heterocycles in heavy crude oils towards benzyl halides.
Schriewer, Alexander	WWU Münster, Deutschland	Online SPE-HILIC-ESI-MS/MS zur Untersuchung des Metabolismus von auf Acetyl-CoA und Malonyl-CoA in MCF-7 Brustkrebszellen Vortragend
Schubert, Ulrich S.	Friedrich Schiller University Jena, Deutschland	Effect of ecosystem type and fire on chemistry of WEOM as measured by LDI-TOF-MS and NMR
Schuhmann, Kai	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Deutschland	Intensity Independent Filtering of FT MS and FT MS/MS Spectra for Shotgun Lipidomics Vortragend Lipidomics reveals lipid networks correlated with the progression of human colorectal cancer
Schulz, Sabine	Justus-Liebig-Universität Gießen, Deutschland	Development of an autarkic desorption electrospray ionization source for in-field DESI-MS applications Real-time food authentication with a miniature mass spectrometer
Schümann, Michael	Leibniz Institut für Molekulare Pharmakologie, Deutschland	Analysis of serine-phosphorylation dependent protein-protein interactions of the T cell adaptor protein ADAP Neutral loss-triggered EThcD mass spectrometry identifies protein pyrophosphorylation in vivo
Schütze, Johannes	IPK-Gatersleben, Deutschland	Characterization of plastidal redox-responses during cold stress acclimation Vortragend
Schwaiger-Hufnagel, Ulrike	Bruker Daltonik GmbH, Bremen, Germany	Enabling High-Confidence Human Endogenous Metabolite Identification via High-Resolution MS/MS Retention-Time Library
Schwemer, Theo	Joint Mass Spectrometry Centre / Chair of Analytical Chemistry, University of Rostock, 18059 Rostock, Germany; HICE - Helmholtz Virtual of Complex Molecular Systems in Environmental Health – Aerosols and Health, www.hice-vi.eu	Evolved gas analysis ultra high resolution mass spectrometry - Insights into heavy petroleum fractions and combustion aerosol
Schwudke, Dominik	Division of Bioanalytical Chemistry, Research Center Borstel, Germany; German Center for Infection Research, Clinical Tuberculosis Center, Borstel, Germany; Research Center Borstel, Division of Bioanalytical Chemistry, Parkallee 1-40, D-23845 Borstel, Germany.; Airway Research Center North, German Center for Lung Research, Wöhrendamm 80, 22927 Großhansdorf, Germany	LC-MS2 Method Development for Simultaneous Analysis of Antibiotics from Plasma of MDR-TB Patients Lipidomes of human lung tissues show distinct lipid metabolic alterations for lung cancer and pulmonary emphysema Lipidomics of Pig Brain Using the PIRL-DIVE Homogenisation Technique Software platform to improve the quality control of Lipid mediator quantification
Seeberger, Peter	Freie Universität Berlin, Deutschland; Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Potsdam, Deutschland	Glycan Fingerprinting using Cold-Ion Infrared Spectroscopy
Seulen, Sarah	Christian-Albrechts-Universität zu Kiel, Deutschland	Untersuchungen zu den unimolekularen und stoßaktivierten Fragmentierungsmechanismen der Diethyltoluidine über Isotopenmarkierungen Vortragend
Shadyro, Oleg	Belarusian State University, Department of Chemistry, Leningradskaya 14, 220006, Minsk, Belarus	Cytochrome c-mediated modification of cardiolipin
Shema, Gerta	ISAS, Deutschland	Simple, scalable and sensitive tip-based enrichment of N-terminal peptides for profiling of protease substrates
Shevchenko, Andrej	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany, Deutschland; MPI-CBG, Dresden, Deutschland	Absolute quantification of core histones in zebrafish embryos by MS Western Improved protocol for recovery of vesicular proteins Intensity Independent Filtering of FT MS and FT MS/MS Spectra for Shotgun Lipidomics Lipidomics reveals lipid networks correlated with the progression of human colorectal cancer

Autor(en)	Organisation(en)	Titel des Beitrags
		Multifaceted Shotgun Vortragend Polyamine modifications in biosilica-associated proteome
Shevchenko, Anna	MPI of Cell Biology and Genetics, Dresden, Germany	Improved protocol for recovery of vesicular proteins
Shilyaev, Nikita	Department of Biochemistry, St. Petersburg State University, Russia	Age-related glycation hotspots in plant proteome
Sickmann, Albert	Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund, Germany; Department of Chemistry, College of Physical Sciences, University of Aberdeen, United Kingdom; Medizinisches Proteom Center, Ruhr Universität Bochum, Germany	Excellent sensitivity through excellent recovery – ERLIC for absolute quantification of low abundant protein phosphorylation events in cancer patient tissue Temporal quantitative phosphoproteomics of ADP stimulation reveals novel central nodes in platelet activation and inhibition Vortragend
Siegert, Markus	Department of Chemistry, Humboldt Universität zu Berlin, Berlin, Germany	Mass spectrometric investigation of N acetylcysteine as a potential scavenger against sulfur mustard Vortragend
Siemers, Adrian	Analytik Jena AG, Jena, Germany	Ultra High Throughput Drug Discovery Screening by MALDI-TOF Mass Spectrometry
Simon, Fabian	Hochschule Mannheim, Deutschland	Derivatization of low-volatile compounds in aqueous solution and analysis by HS-GC-IMS
Sinz, Andrea	Martin-Luther Universität Halle-Wittenberg, Institute of Pharmacy; Institute of Pharmacy, Martin Luther University Halle-Wittenberg; 1Department of Pharmaceutical Chemistry and Bioanalytics, Institute of Pharmacy, Martin-Luther University Halle-Wittenberg, Halle (Saale), Germany; Martin-Luther-University Halle-Wittenberg, Institute of Pharmacy, Department of Pharmaceutical Chemistry and Bioanalytics, Germany	Age-related formation of advanced glycation end products (AGEs) in root nodules of common beans (Phaseolus vulgaris) Age-related glycation hotspots in plant proteome An Integrated Mass Spectrometry Based Approach to Probe the Structure of the Full-Length Wild-Type Tetrameric p53 Tumor Suppressor An Integrated Workflow for Structural Proteomics Studies based on Cross-linking/Mass Spectrometry with an MS/MS Cleavable Cross-linker Cross-Linking and Mass Spectrometry Shed New Light on the bMunc13-2/Calmodulin Interaction Dissociation behavior of a TEMPO-benzyl cross-linker for peptide structure analysis by free radical initiated peptide sequencing (FRIPS) in negative ESI-MS Mass Spectrometry-Based Interaction Studies of the N-Terminus of the Formate Channel FocA from Escherichia coli Simulated microgravity triggers transient enhancement of protein glycation and oxidation in germinating Brassica napus seeds Structural Insights into Retinal Guanylyl Cyclase/GCAP-2 Interaction by Cross-linking and Mass Spectrometry Synthesis of Isotope-Labeled Derivatives of the MS/MS-Cleavable Urea-Cross-Linker: Synthesis and Evaluation of Reactivity for Effective Protein Structure Analysis
Sklorz, Martin	Universität Rostock, Deutschland; Joint Mass Spectrometry Centre / Chair of Analytical Chemistry, University of Rostock, 18059 Rostock, Germany	Direct resonance-enhanced multi-photon ionisation (REMPI) of complex liquid samples under vacuum conditions Evolved gas analysis ultra high resolution mass spectrometry - Insights into heavy petroleum fractions and combustion aerosol Multiple analysis of individual airborne aerosol particles by laser mass spectrometry: Detection of polyaromatic hydrocarbons from the particle-surface and particle-core Thermal and laser desorption atmospheric pressure photo ionisation ultra high resolution mass spectrometry – Concept and application towards complex samples
Slowik, Jay	Paul Scherrer Institute (PSI), Villigen, Switzerland	Characterization of a New Extractive Electrospray Ionization (EESI) Source for Online Particle Analysis and its Application to Atmospheric Aerosol
Smolikova, Galina	Department of Plant Physiology and Biochemistry, St. Petersburg State University, Russia	Age-related glycation hotspots in plant proteome Profiles of glycated amino acid adducts in the protein hydrolyzates of pea (Pisum sativum) seeds subjected to accelerated ageing Simulated microgravity triggers transient enhancement of protein glycation and oxidation in germinating Brassica napus seeds
Soboleva, Alena	Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry, Germany; Department of Biochemistry, St. Petersburg State University, Russia	Profiles of glycated amino acid adducts in the protein hydrolyzates of pea (Pisum sativum) seeds subjected to accelerated ageing

Autor(en)	Organisation(en)	Titel des Beitrags
Sobott, Frank	Universiteit Antwerpen, Belgien	Formation and Properties of a Compact Protein Unfolding Intermediate in the Gas-phase
Solari, Fiorella A.	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Deutschland	Temporal quantitative phosphoproteomics of ADP stimulation reveals novel central nodes in platelet activation and inhibition
Soltwisch, Jens	University of Münster, Insitute for Hygiene, Münster, Germany; Interdisciplinary Center for Clinical Research (IZKF) Münster, Germany; Institute for Hygiene, Biomedical Mass Spectrometry, University of Münster, Germany; Institute for Hygiene, University of Münster, Robert-Koch-Str. 41, 48149 Münster, Germany	CoolMALDI: Combination of IR-ablation and UV-postionization of snap-frozen tissue sections for sensitive imaging of lipids and metabolites Vortragend New insights into the MALDI mechanisms: Postionization and photoacoustic experiments reveal laser spot size-dependent transitions between desorption and ablation regimes The internal energy in a MALDI plume probed with thermometer molecules: Effects of laser excitation wavelength and laser fluence Towards qMALDI-MSI : MS imaging of phospholipids in mouse cerebellum followed by semi-quantitative nano-HPLC-ESI-MS of extracts from laser micro-dissected brain regions Colorful MALDI: Effect of the Laser Excitation Wavelength on the Analytical Sensitivity in Standard MALDI-MS and Imaging Experiments Micro-arrays of faux tissue to investigate ion suppression effects in MALDI mass spectrometry of lipids
Spengler, Bernhard	Justus-Liebig-Universität Gießen, Institut für Anorganische und Analytische Chemie; Institute of Inorganic and Analytical Chemistry, Justus-Liebig-University, Giessen, Germany; Justus-Liebig-Universität Gießen, Deutschland; Justus Liebig University Giessen, Germany	AP-SMALDI MSI of metabolites and lipids in Schistosoma mansoni parasites Charge Switching of Phospholipids using Paternó-Büchi Reactions Development of an autarkic desorption electrospray ionization source for in-field DESI-MS applications Differentiating wild and mutant C. elegans using high-resolution atmospheric pressure matrix assisted laser desorption/ionization mass spectrometry imaging Imaging metabolites in wheat stem base-Fusarium graminearum interactions using high-resolution atmospheric pressure scanning microprobe MALDI mass spectrometry imaging (SMALDI-MSI) Implementation of a High Repetition-Rate Laser System in an AP-SMALDI MSI System for Enhanced Measurement Speed Implementation of Ultraviolet Photodissociation on a LTQ FT Ultra Mass Spectrometer and first Applications Optimization of the LAMPAS 3 laser mass spectrometer for improved on-line single particle analysis Rapid fingerprinting of lignin renewable energy sources by ambient ionization high-resolution mass spectrometry and simplified data mining Reactive low temperature plasma (LTP) mass spectrometry of neurosteroids Real-time food authentication with a miniature mass spectrometer Resolution enhancement by delayed ion extraction in a single-particle aerosol mass spectrometer
Sperling, Michael	Institute of Inorganic and Analytical Chemistry, University of Münster, Münster, Germany; European Virtual Institute for Speciation Analysis (EVISA), Münster, Germany; Westfälische Wilhelms-Universität Münster	Elemental Bioimaging by LA-ICP-QQQ-MS for the Investigation of Wilson´s Disease Imaging of Cerium Oxide Nanoparticles and Phospholipids in Rat Lung Tissue by Means of LA-ICP-MS and MALDI-MS
Spiteller, Peter	Universität Bremen, Deutschland	Separation and identification of muscarine isomers
Springer, Andreas	Freie Universität Berlin, Institute of Chemistry and Biochemistry, Core Facility BioSupraMol	UPLC-ESI-QTOF-MS based chemical profiling of Actaea racemosa L. (black cohosh) rhizomes to investigate differences in cultivation, wild harvest, and genotypes
Stafford, George	Agilent Technologies, Santa Clara, USA	Standardised Collision Cross Section Measurements by Single Static Drift Field Ion Mobility Instrument in an Interlaboratory Study
Stark, Tina	Goethe-Universität Frankfurt, Deutschland	Steps towards a more native analysis of Aß42 using LILBID mass spectrometry
Steffen, Bernhard	Forschungszentrum Jülich, Deutschland	Historical charcoal additions potentially improve stability of soil organic carbon
Steffen, Pascal	University Medical Center Hamburg-Eppendorf, Deutschland	Comparison of Data-Independent Acquisition (DIA) and Data-Dependent Acquisition (DDA) for label-free Quantification Vortragend Comparison of label free quantification methods for proteomics Mass spectrometric characterization of aberrant O-glycosylation in COSMC deficient mouse pancreas tissue

Autor(en)	Organisation(en)	Titel des Beitrags
Stephanowitz, Heike	Leibniz Institut für Molekulare Pharmakologie, Deutschland	Analysis of serine-phosphorylation dependent protein-protein interactions of the T cell adaptor protein ADAP
Stöcker, Winfried	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	The role of mass spectrometry in the identification of autoantigens as targets in neurological autoimmune diseases
Stokes, Caroline	Universitätsklinikum des Saarlandes, Homburg, Deutschland	Vitamin D3 epimers: analytical nuisance or clinical opportunity?
Stow, Sarah	Vanderbilt University, USA	Standardised Collision Cross Section Measurements by Single Static Drift Field Ion Mobility Instrument in an Interlaboratory Study
Streibel, Thorsten	Universität Rostock, Deutschland; Helmholtz-Zentrum München,Deutschland	Thermogravimetry coupled to Ultrafast Gas Chromatography Singlephoton-Ionisation Time-of-Flight-Mass-Spectrometry (TG-SPI-TOF-MS) for Evolved-Gas-Analysis of Fuels regarding to the Deposit Formation Potential
Striegel, Lisa	Technische Universität Münschen, Lehrstuhl für Analytische Lebensmittelchemie	Validierung einer Stabilisotopenverdünnungsanalyse von Folaten in Lebensmitteln und Bestimmung des Folatgehaltes in Naturprodukten
Struwe, Weston B.	Oxford Glycobiology Institute, Universität Oxford, Oxford, UK	Glycan Fingerprinting using Cold-Ion Infrared Spectroscopy
Stummer, Walter	University Hospital of Münster, Department of Neurosurgery, Münster, Germany	Bioimaging of photosensitizers in human brain tumors after fluorescence-guided resection
Sturm, Patrick	TOFWERK, Switzerland	Determination of multi-element composition and mass of single nanoparticles in liquids and air
Stützer, Alexandra	Max Planck Institute for Biophysical Chemistry, Göttingen, Germany	Analysis of UV-induced DNA–protein cross-links in a chromatin model Vortragend Analysis of 1,2,3,4-diepoxybutane induced DNA-histone cross-links by mass spectrometry
Suckau, Detlev	Bruker Daltonik GmbH, Deutschland	The Next Generation Ion Mobility Separation (IMS) Adds A New Dimension to Substance Characterization and Identification Vortragend
Süß, Rosmarie	University of Leipzig, Medical Faculty, Institute of Medical Physics and Biophysics	Differentiation and relative quantification of chondroitin sulfate isomers by ion mobility spectrometry-mass spectrometry and pulsed-field gradient NMR
Sutton, Jennifer	Thermo Fisher Scientific, USA	Full Characterization of Antibodies Under Denaturing and Native Conditions on a Hybrid Quadrupole-Orbitrap MS Equipped With a Higher Mass Range
Svatoš, Aleš	Max Planck Institute for Chemical Ecology, Jena, Germany; Institute of Organic Chemistry and Biochemistry, AS CR, Prague, Czech Republic; Research Group Mass spectrometry/Proteomics, Max Planck Institute for Chemical Ecology	Application of high-throughput MS screening to disentangle the bacterial metabolome Application of the Superbasic Matrix DPN in Atmospheric Pressure MALDI-MS-Analyses of Biological Samples Mapping metabolites from rough terrain: laser ablation electrospray ionization on non-flat samples
Szesny, Matthias	Bruker Daltonik GmbH, Deutschland	Boosting compound identification confidence in Metabolomics by exploiting all available Q-TOF high resolution accurate mass spectral information. Vortragend Increasing arginine production in C. glutamicum by rational strain design using a combination of metabolomics and proteomics Vortragend Investigation of Q-TOF instruments advantages for label-free proteome analysis Vortragend Metabolomics to study the “war” between plants and insects - Systemic defense induction and post-ingestive rearrangement of plant toxins in insects. Vortragend
Tampé, Robert	Johann Wolfgang Goethe-Universität, Deutschland	Analyzing macromolecular complexes: subunit interactions of the F1F0 ATP synthase and conformational changes of the heterodimeric ABC transport complex TmrAB
Tanner, Martin	TOFWERK, Switzerland	Determination of multi-element composition and mass of single nanoparticles in liquids and air
Tarakhovskaya, Elena	Department of Plant Physiology and Biochemistry, St. Petersburg State University, Russia;	Age-related glycation hotspots in plant proteome Application of LC-MS technique for intra-thallus profiling of polyphenolics in three species of fucoid algae Vortragend

Autor(en)	Organisation(en)	Titel des Beitrags
	St-Petersburg State University, Russia	
Tatlay, Jaspaul	Department of Chemistry, University of Alberta, Edmonton, Canada	Enabling High-Confidence Human Endogenous Metabolite Identification via High-Resolution MS/MS Retention-Time Library
Teegen, Bianca	Institute for Experimental Immunology, affiliated to EUROIMMUN AG, Luebeck, Germany	The role of mass spectrometry in the identification of autoantigens as targets in neurological autoimmune diseases
Temporini, Caterina	Department of Drug Sciences, University of Pavia, Pavia, Italy	Innovative analytical methodologies for the development of new antitubercular agents
Tengattini, Sara	Department of Drug Sciences, University of Pavia, Pavia, Italy	Innovative analytical methodologies for the development of new antitubercular agents
Thiele, Björn	IBG-2 Pflanzenwissenschaften, Forschungszentrum Jülich, Deutschland	Quantitative turnover analysis of chlorophylls, carotenoids and tocopherol in green leaves by LC-MS and FTICR-MS Vortragend
Thiermann, Horst	Bundeswehr Institute of Pharmacology and Toxicology	Albumin adducts as biomarkers of an exposure with organophosphorus pesticides Mass spectrometric investigation of N acetylcysteine as a potential scavenger against sulfur mustard
Thiesen, Hans-Jürgen	Institute of Immunology, University of Rostock, Germany	Intact Transition Epitope Mapping - A mass spectrometric method for accurate, facile, and rapid identification of specific antibody-peptide reactivities
Tholey, Andreas	Div. Systematic Proteome Research & Bioanalytics, Institute for Experimental Medicine, Kiel University, Germany; Institut für Experimentelle Medizin, Uni Kiel; Christian-Albrechts-Universität zu Kiel, Deutschland	Combining 2D-LC-MS and Gelfree-LC-MS enhances both proteome coverage and the identification of short open reading frame encoded peptides Identification and characterization of N-acyl homoserine lactones by mass spectrometry Identification and classification of amyloidosis by matrix-assisted laser desorption/ionization mass spectrometry imaging Identification and quantification of N-acyl homoserine lactones involved in bacterial communication by matrix-assisted laser desorption/ionization mass spectrometry Improving the sequence coverage in top-down MS/MS of proteins Quantitative proteomics for the analysis of molecular changes in lung adenocarcinoma cells in response to Vitamin D3
Thomas, Daniel A.	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland	Glycan Fingerprinting using Cold-Ion Infrared Spectroscopy
Thomas, Henrik	MPI of Cell Biology and Genetics, Dresden, Germany	Improved protocol for recovery of vesicular proteins Intensity Independent Filtering of FT MS and FT MS/MS Spectra for Shotgun Lipidomics
Thompson, Christopher	Bruker Daltonics, Billerica, MA, USA	MALDI FT-ICR Imaging: Double the Performance or Double the Samples using Quadrupolar Detection
Thompson, Christopher J.	Bruker Daltonics Inc., Billerica, MA, USA	2ω-FT-ICR Mass Spectrometry with Quadrupolar Detection
Tissier, Alain	Department of Cell and Metabolic Biology, Leibniz Institute of Plant Biochemistry (Halle/Saale)	Age-related glycation hotspots in plant proteome
Torres, Tomás	Universidad Autónoma de Madrid, Spain; Instituto Madrileño de Estudios Avanzados (IMDEA)-Nanociencia, Spain	Aggregation of a crown-ether decorated zinc-phthalocyanine by collision-induced desolvation providing insight into the electrospray mechanism
Totzeck, Matthias	University Hospital Essen, Medical Faculty, West German Heart and Vascular Center, Department of Cardiology and Department of Angiology, Germany	SIMPLEX reveals myoglobin as a key player in cardiac lipid metabolism
Towers, Mark	Waters Corporation, United Kingdom	Getting DESI Imaging up to speed for clinical applications
Traikov, Sofia	MPI of Cell Biology and Genetics, Dresden, Germany	Improved protocol for recovery of vesicular proteins Vortragend
Treitz, Christian	Institut für Experimentelle Medizin, Uni Kiel; AG Systematische Proteomforschung &	Identification and characterization of N-acyl homoserine lactones by mass spectrometry Vortragend Identification and quantification of N-acyl homoserine lactones

Autor(en)	Organisation(en)	Titel des Beitrags
	Bioanalytik, Institut für Experimentelle Medizin, Christian-Albrechts-Universität zu Kiel, Kiel, Deutschland	involved in bacterial communication by matrix-assisted laser desorption/ionization mass spectrometry
Treu, Axel	Universität Bayreuth, Deutschland	Multimodal imaging combining mass spectrometry and vibrational spectroscopy using a single tissue section and an integrated data processing workflow Vortragend Separation and identification of muscarine isomers
Trog, Sabrina	Humboldt-Universität zu Berlin, Deutschland	Mass Spectrometry Imaging as Tool for the Analysis of MRI Contrast Agents in Biological Tissues Vortragend
Tudzynski, Paul	Institute of Plant Biology and Biotechnology, University of Münster, Germany	Localization of Ergot Alkaloids in Sclerotia of Claviceps purpurea by MALDI-MS Imaging
Turunen, Lotta	Department of Chemistry, NanoScience Center, University of Jyvaskyla, Finnland	Investigation of Dimeric and Hexameric Halogen-Bonded Supramolecular Capsules by ESI-MS and IM-MS
Tyrasa, Swen	Analytik Jena AG, Jena, Germany	Ultra High Throughput Drug Discovery Screening by MALDI-TOF Mass Spectrometry
Uecker, Marina	Proteomics Group, Max-Planck-Institute of Experimental Medicine, 37075 Göttingen, Germany	Partial Immunoblotting of 2D-Gels: A Novel Method to Identify Post-Translationally Modified Proteins Exemplified for the Myelin Acetylome
Uetrecht, Charlotte	Heinrich-Pette-Institut, Hamburg, Deutschland; European XFEL GmbH, Schenefeld, Germany; Heinrich Pette Institute, Leibniz Institute for Experimental Virology, Hamburg, Germany	Analyzing self-assembly of Ebola virus nucleoprotein with native mass spectrometry Native mass spectrometry analysis of norovirus - glycan mimetics interaction Structural characterization of protein-lipid complexes involved in clathrin-mediated endocytosis Studying viral capsid glycan interaction with native MS
Uhl, Agnes	Friedrich-Alexander-University Erlangen-Nürnberg, Germany	Reactivity and stability check of even vs. odd electron (quasi)-molecular ions derived from triangulenium type derivatives
Ulbrich, Anne	Universität Rostock, Deutschland	Thermogravimetry coupled to Ultrafast Gas Chromatography Singlephoton-Ionisation Time-of-Flight-Mass-Spectrometry (TG-SPI-TOF-MS) for Evolved-Gas-Analysis of Fuels regarding to the Deposit Formation Potential Vortragend
Urlaub, Henning	Bioanalytical Mass Spectrometry, Max Planck Institute for Biophysical Chemistry, Göttingen, Germany; University Medical Center Göttingen, Germany	Analysis of 1,2,3,4-diepoxybutane induced DNA-histone cross-links by mass spectrometry Analysis of UV-induced DNA–protein cross-links in a chromatin model
Uschold, Stephanie	Max Planck Institute for the Structure and Dynamics of Matter CFEL, Hamburg	Proteomic investigation of skin cell layers by tissue ablation using picosecond infrared laser (PIRL)
Van Orden, Steve L.	Bruker Daltonics Inc., Billerica, MA, USA	2ω-FT-ICR Mass Spectrometry with Quadrupolar Detection
Van Soest, Remco	SCIEX, USA	Accelerating Data Independent Acquisition with Microflow Chromatography
VanOrden, Steve	Bruker Daltonics, Billerica, MA, USA	MALDI FT-ICR Imaging: Double the Performance or Double the Samples using Quadrupolar Detection
Vappiani, Johanna	Cellzome GmbH, Heidelberg	Analysis of drug-induced effects on proteostasis in cell lines and non-dividing primary cells by quantitative mass spectrometry
Vastenhouw, Nadine	Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany, Deutschland	Absolute quantification of core histones in zebrafish embryos by MS Western
Vaudel, Marc	KG Jebsen Center for Diabetes Research, Department of Clinical Science, University of Bergen, Norway; Center for Medical Genetics and Molecular Medicine, Haukeland University Hospital, Bergen, Norway	PeptideMapper: Efficient and Versatile Amino Acid Sequence and Tag Mapping
Vendruscolo, Michele	University of Cambridge, United Kingdom	Steps towards a more native analysis of Aß42 using LILBID mass spectrometry

Autor(en)	Organisation(en)	Titel des Beitrags
Venne, A. Saskia	ISAS, Deutschland	Simple, scalable and sensitive tip-based enrichment of N-terminal peptides for profiling of protease substrates
Vennemann, Antje	IBE R&D gGmbH	Imaging of Cerium Oxide Nanoparticles and Phospholipids in Rat Lung Tissue by Means of LA-ICP-MS and MALDI-MS
Vens-Cappell, Simeon	University of Münster, Insitute for Hygiene, Münster, Germany; Interdisciplinary Center for Clinical Research (IZKF) Münster, Germany	CoolMALDI: Combination of IR-ablation and UV-postionization of snap-frozen tissue sections for sensitive imaging of lipids and metabolites Localization of Ergot Alkaloids in Sclerotia of Claviceps purpurea by MALDI-MS Imaging Vortragend
Verhelst, Steven	ISAS, Deutschland; Department of Cellular and Molecular Medicine, Leuven, Belgium	Simple, scalable and sensitive tip-based enrichment of N-terminal peptides for profiling of protease substrates
Vetere, Alessandro	Max-Planck-Institut für Kohlenforschung, Deutschland	APPI-FAIMS-FTMS source and electrode optimization for the elucidation of structural features of crude oil constituents Vortragend
Vialaret, Jerome	Laboratoire de Biochimie et Protéomique Clinique, Institut de Médecine Régénératrice et de Biothérapie, CHU de Montpellier - Hôpital St. Eloi, Montpellier, France	Applying a Proteoform profiling method for neurological disorder biomarker discovery operations
Vikhnina, Maria	Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry, Germany; Department of Biochemistry, St. Petersburg State University, Russia	Profiles of glycated amino acid adducts in the protein hydrolyzates of pea (Pisum sativum) seeds subjected to accelerated ageing Vortragend
Villatoro, José	University of Potsdam, Germany; Bundesanstalt für Materialforschung und -prüfung, Germany; School of Analytical Sciences Adlershof, Germany	IR-MALDI Ion Mobility Spectrometry: Low and High Field Mobilities of Peptide Ions at Intermediate Pressure Vortragend
Viner, Rosa	Thermo Fisher Scientific, San Jose, CA, USA	Optimization of crosslinked peptide analysis on an Orbitrap Fusion Lumos mass spectrometer
Vissers, Johannes PC	Waters Corporation, Wilmslow, United Kingdom	IMS-DIA-MS Characterisation and IMS-MRM QconCAT Quantitation of the Lipidome and Apolipoprotein Complements of Obesity and Diabetes Cohorts Quantitation of Proteomics Samples Using a Novel Scanning Quadrupole DIA Method
Vitt, Stella	Max Planck Institute of Biophysics, Frankfurt	From Salty to Salt-free: Monitoring the Salt-dependent Dissoziation of the Membrane Protein Complex GCD in a Single Experiment
Vitz, Jürgen	Friedrich Schiller University Jena, Deutschland	Effect of ecosystem type and fire on chemistry of WEOM as measured by LDI-TOF-MS and NMR
Vogel, Sarah	Institute of Physiological Chemistry, Faculty of Medicine Carl Gustav Carus, Technical University Dresden, Germany	Comparative analysis of the effects of sulfated hyaluronic acid and dexamethasone on osteoblast differentiation by nanoLC-MS and random forest modeling.
Vogt, Thomas	Department of Cell and Metabolic Biology, Leibniz Institute of Plant Biochemistry (Halle/Saale)	Age-related glycation hotspots in plant proteome
Volmer, Dietrich A.	Saarland University, Saarbrücken, Deutschland	Rapid fingerprinting of lignin renewable energy sources by ambient ionization high-resolution mass spectrometry and simplified data mining Vitamin D3 epimers: analytical nuisance or clinical opportunity? Vortragend Direct aqueous measurement of 25-hydroxyvitamin D in cellular environments by LC-MS/MS using the novel chemical derivatization reagent MDBP
von Bergen, Martin	Department for Molecular Systems Biology, Helmholtz Centre for Environmental Research – UFZ, Leipzig, Germany; Institute of Biochemistry, Faculty of Biosciences, Pharmacy and Psychology,	Comparative analysis of the effects of sulfated hyaluronic acid and dexamethasone on osteoblast differentiation by nanoLC-MS and random forest modeling. Phthalate metabolites MEHP and MEOHP but not the phthalate DEHP itself bind and activate the PPARγ

Autor(en)	Organisation(en)	Titel des Beitrags
	University of Leipzig, Germany; Helmholtz-Centre for Environmental research (UFZ), Department of Molecular Systems Biology, Leipzig, Germany	
von der Wellen, Jens	Bundeswehr Institute of Pharmacology and Toxicology	Albumin adducts as biomarkers of an exposure with organophosphorus pesticides Vortragend
von Helden, Gert	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland	Glycan Fingerprinting using Cold-Ion Infrared Spectroscopy The Amyloid Formation Mechanism of Human IAPP: An Infrared Spectroscopy Approach
Vosse, Christian	Westfälische Wilhelms-Universität Münster, Deutschland	Profiling von konfigurationsisomeren Phospholipiden mittels HILIC-ESI-MS/MS Vortragend
Vu Huu, Khanh	Johann Wolfgang Goethe-Universität, Deutschland	Analyzing macromolecular complexes: subunit interactions of the F1F0 ATP synthase and conformational changes of the heterodimeric ABC transport complex TmrAB Vortragend
Wachsmuth, Christian J.	University of Regensburg, Institute of Functional Genomics, Regensburg, Deutschland	A step forward in GC-HRAM-MS based metabolomics - A novel atmospheric pressure GC-APCI Source increases quantitative and qualitative performance
Wagner, Anne	Cellzome GmbH, Heidelberg	Analysis of drug-induced effects on proteostasis in cell lines and non-dividing primary cells by quantitative mass spectrometry
Walter, Frederik	Bielefeld University, Bielefeld, Deutschland	Boosting compound identification confidence in Metabolomics by exploiting all available Q-TOF high resolution accurate mass spectral information.
Walter, Ulrich	Center for Thrombosis and Hemostasis, Universitätsklinikum der Johannes Gutenberg-Universität Mainz, Mainz, Germany;	Temporal quantitative phosphoproteomics of ADP stimulation reveals novel central nodes in platelet activation and inhibition
Walters, David	Fort Collins Science Center, US Geological Survey, Fort Collins, USA	Investigating the zinc distribution in the mayfly N. triangulifer using elemental bioimaging by LA-ICP-MS
Wanczek, Karl Peter	Universität Bremen	Power-function Resolution Filter in Fourier Transform Mass Spectrometry
Wang, Nan	Department of Chemistry, University of Alberta, Edmonton, Canada	Enabling High-Confidence Human Endogenous Metabolite Identification via High-Resolution MS/MS Retention-Time Library
Wang, Qing	Department of Plant Breeding, Justus Liebig University Giessen, Heinrich-Buff-Ring 26–32, 35392 Giessen, Germany	Imaging metabolites in wheat stem base-Fusarium graminearum interactions using high-resolution atmospheric pressure scanning microprobe MALDI mass spectrometry imaging (SMALDI-MSI)
Wang, Xiaohang	Department of Chemistry, University of Alberta, Edmonton, Canada	Enabling High-Confidence Human Endogenous Metabolite Identification via High-Resolution MS/MS Retention-Time Library
Wang, Xuxiao	Max-Planck-Institut für Kohlenforschung, Deutschland	Electrospray Fourier Transform ion cyclotron resolution mass spectrometry: reactivity of polyaromantic heterocycles in heavy crude oils towards benzyl halides. Vortragend
Wang, Yuting	Center for Regenerative Therapies, Technical University Dresden, Dresden, Germany; Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany	Lipidomics reveals lipid networks correlated with the progression of human colorectal cancer Vortragend
Warmbrunn, Vera	Friedrich-Alexander-University Erlangen-Nürnberg, Germany	Formation and structure elucidation of $[M_2$ and $Ag]^+$ ions with M = [6]helicene, [7]helicene and coronene Vortragend
Warzok, Ulrike	Freie Universität Berlin	Investigation of Dimeric and Hexameric Halogen-Bonded Supramolecular Capsules by ESI-MS and IM-MS Vortragend
Watz, Henrik	Pulmonary Research Institute at LungenClinic Großhansdorf, Wöhrendamm 80, 22927 Großhansdorf.; Airway Research Center North, German Center for	Lipidomes of human lung tissues show distinct lipid metabolic alterations for lung cancer and pulmonary emphysema

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	Lung Research, Wöhrendamm 80, 22927 Großhansdorf, Germany	
Weber, Marcus	Zuse Institute Berlin, Germany	IR-MALDI Ion Mobility Spectrometry: Low and High Field Mobilities of Peptide Ions at Intermediate Pressure
Weibchen, Gunnar	Waters GmbH, Germany	Increased confidence for the identification of N-linked glycopeptides using an optimised collision energy workflow Vortragend Lipidomics Quantitation Using a Novel Scanning Quadrupole DIA Method Vortragend
Weinmann, Wolfgang	Institute of Forensic Medicine, University of Bern; University of Bern, Institute of Forensic Medicine, Forensic Toxicology and Chemistry, Bühlstrasse 20, 3012 Bern, Switzerland; Universtität Bern, Institut für Rechtsmedizin, Forensische Toxikologie und Chemie, Switzerland	N-Acetyltaurine as a novel urinary ethanol marker in a drinking study Separation of isomeric cannabinoids by high-resolution ion mobility-MS for the differentiation of legal and illegal marijuana Update of an MS/MS Library of NPS for QTRAP® instruments
Weissflog, Jerrit	Max Planck Institute for Chemical Ecology, Jena, Germany	Application of the Superbasic Matrix DPN in Atmospheric Pressure MALDI-MS-Analyses of Biological Samples Vortragend
Weller, Philipp	Hochschule Mannheim, Deutschland	Derivatization of low-volatile compounds in aqueous solution and analysis by HS-GC-IMS Quality assessment of olive oil based on volatile compound fingerprinting using HRGC-IMS analysis
Wendt, Juergen	LECO European Application&Technology Center, Berlin, Germany	The Usage of Direct Inlet Probe in combination with High Resolution Mass Spectrometry Vortragend The Usage of Direct Inlet Probe in combination with High Resolution Mass Spectrometry for the Characterization of Heavy Petroleum Products
Wendt, Karin	Bruker Daltonik GmbH, Deutschland	Simultaneous quantitation and confirmation of about 500 pesticide residues in food extracts using LC-QTOF accurate mass spectrometry
Werner, Hauke	Department of Neurogenetics, Max-Planck-Institute of Experimental Medicine, 37075 Göttingen, Germany	Partial Immunoblotting of 2D-Gels: A Novel Method to Identify Post-Translationally Modified Proteins Exemplified for the Myelin Acetylome
Weske, Sebastian	Georg-August-University Göttingen, Germany	Coinage-Metal Ate Complexes – An ESI-MS Study Vortragend
Wessjohann, Ludger A.	Leibniz Institute of Plant Biochemistry, Department of Bioorganic Chemistry; Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry (Halle/Saale); Leibniz-Institut für Pflanzenbiochemie, Abteilung Natur- und Wirkstoffchemie, Germany	Age-related formation of advanced glycation end products (AGEs) in root nodules of common beans (Phaseolus vulgaris) Age-related glycation hotspots in plant proteome Probing plant Maillard reaction by mass spectrometry in model peptide systems
Westphal, Dennis	Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Universität Leipzig, Germany	Identification of oxidative biomarkers in synovial fluid of patients suffering from rheumatoid arthritis Vortragend
Widdig, Anja	Universität Leipzig, Deutschland; Max-Planck-Institut für Evolutionäre Anthropologie, Leipzig, Deutschland; Deutsches Zentrum für integrative Biodiversitätsforschung, Leipzig, Deutschland; German Center for Integrative Biodiversity Research (iDiv), Germany	The performance of mobile GC-MS for field sampling of body odours from common marmosets (Callithrix jacchus) Methodological aspects of mass spectrometric detection for profiling ambient VOCs with thermodesorption-GCMS
Wiegelmann, Marcel	Institute for Hygiene, Biomedical Mass	New insights into the MALDI mechanisms: Postionization and photoacoustic experiments reveal laser spot size-dependent transitions between desorption and ablation regimes Vortragend

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	Spectrometry, University of Münster, Germany	Micro-arrays of faux tissue to investigate ion suppression effects in MALDI mass spectrometry of lipids
Wiemann, Martin	IBE R&D gGmbH	Imaging of Cerium Oxide Nanoparticles and Phospholipids in Rat Lung Tissue by Means of LA-ICP-MS and MALDI-MS
Wildgoose, Jason	Waters Corporation, Wilmslow, United Kingdom	Lipidomics Quantitation Using a Novel Scanning Quadrupole DIA Method Quantitation of Proteomics Samples Using a Novel Scanning Quadrupole DIA Method
Wilharm, Thomas	ASG Analytik Service-Gesellschaft mbH, Neusäss	The Usage of Direct Inlet Probe in combination with High Resolution Mass Spectrometry for the Characterization of Heavy Petroleum Products
Winter, Martin	Institute of Pathology, Christian-Albrechts-Universität, Kiel, Germany	Identification and classification of amyloidosis by matrix-assisted laser desorption/ionization mass spectrometry imaging Vortragend
Witt, Matthias	Bruker Daltonik GmbH, Bremen, Germany	2ω-FT-ICR Mass Spectrometry with Quadrupolar Detection MALDI FT-ICR Imaging: Double the Performance or Double the Samples using Quadrupolar Detection
Wittig, Ilka	Goethe-Universität-Frankfurt	ArgC-like digestion: complementary or alternative to tryptic digestion?
Wittig, Sabine	Interdisciplinary research center HALOmem, Martin Luther University Halle-Wittenberg, Kurt-Moses-Straße-3, 06120 Halle (Saale).	Development of a protein interaction networks in synaptic vesicles using cross-linking and mass spectrometry Vortragend
Wohlfahrt, Sebastian	Helmholtz-Zentrum München,Deutschland	Thermogravimetry coupled to Ultrafast Gas Chromatography Singlephoton-Ionisation Time-of-Flight-Mass-Spectrometry (TG-SPI-TOF-MS) for Evolved-Gas-Analysis of Fuels regarding to the Deposit Formation Potential
Wolf, Rainer	Competence Center Analytics, BASF SE, D-67056 Ludwigshafen	Determination of Molecular Formulas from Complex Isotope Pattern Vortragend
Wolters-Eisfeld, Gerrit	University Medical Center Hamburg-Eppendorf, Deutschland	Application of laser ablation for tissue metabolomics Mass spectrometric characterization of aberrant O-glycosylation in COSMC deficient mouse pancreas tissue
Woolerton, Yvonne	Centre for Proteome Research, Institute of Integrative Biology, University of Liverpool, Liverpool, UK	IMS-DIA-MS Characterisation and IMS-MRM QconCAT Quantitation of the Lipidome and Apolipoprotein Complements of Obesity and Diabetes Cohorts
Wozny, Katharina	Biochemie-Zentrum Heidelberg, Deutschland	Quantitative Positional Isomer Analysis of Mixed Diacyl-Glycerophospholipids (dGPLs) by Ultra Performance Liquid Chromatography-Electrospray-Tandem Mass Spectrometry (UPLC-ESI-MS/MS) Vortragend Spotting of Structural Isomer Mixtures of Diacyl-Glycerophospholipids via UPLC-MS/MS
Wrage, Jasmin	GALAB Laboratories GmbH, Deutschland	Discrimination of apple and potato cultivars by non-targeted metabolomic fingerprinting via UPLC-IMS-QToF analysis Vortragend
Wu, Yiman	Department of Chemistry, University of Alberta, Edmonton, Canada	Enabling High-Confidence Human Endogenous Metabolite Identification via High-Resolution MS/MS Retention-Time Library
Wulf, Helena	Universitätsklinikum Schleswig-Holstein, Deutschland	Entwicklung einer LC-MS/MS Methode zur Bestimmung der Backdoorpathway Hormone Androsterone und Androstandiol und der Androgene Androstendion, Testosteron und Dihydrotestosteron
Wurlitzer, Marcus	University Medical Centre Hamburg-Eppendorf, Institute of Clinical Chemistry, Department for Mass Spectrometric Proteomics, Hamburg Germany	Lipidomics of Pig Brain Using the PIRL-DIVE Homogenisation Technique
Wutkowski, Adam	Division of Bioanalytical Chemistry, Research Center Borstel, Parkallee 10, Borstel, Germany	Software platform to improve the quality control of Lipid mediator quantification Vortragend
Xu, Xiaoma	Netherlands Forensic Institute, Forensic Chemistry – Chemical Identification Analysis, 2497 GB The Hague, Netherlands	Development and implementation of new analytical methods and databases for the detection of additives in fuels and fire debris.
Xu, Yun	Max-Planck-Institut für Kohlenforschung, Deutschland	Characterization of Fast-Pyrolysis Bio-Oil Vortragend

Autor(en)	Organisation(en)	Titel des Beitrags
Yan, Hao	Heinrich Pette Institute, Leibniz Institute for Experimental Virology, Hamburg, Germany	Native mass spectrometry analysis of norovirus - glycan mimetics interaction Vortragend Studying viral capsid glycan interaction with native MS
Yates, Lisa M.	Princeton University	Neutral loss-triggered EThcD mass spectrometry identifies protein pyrophosphorylation in vivo
Yavor, Mikhail	Institute of Analytical instrumentation, Russian Academy of Sciences, Russia	Tandem Mass Spectrometry with a (Ultra-)High Resolving Time-of-Flight Mass Spectrometer
Yefremova, Yelena	Proteome Center Rostock, Deutschland	Intact Transition Epitope Mapping - A mass spectrometric method for accurate, facile, and rapid identification of specific antibody-peptide reactivities
Young, Phoebe	Goethe Universität Frankfurt, Deutschland	Characterizing the LILBID ionization method: energy transfer and dissociation Vortragend
Zahedi, René	Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund, Germany	Excellent sensitivity through excellent recovery – ERLIC for absolute quantification of low abundant protein phosphorylation events in cancer patient tissue
Zahedi, René P.	ISAS, Deutschland	Simple, scalable and sensitive tip-based enrichment of N-terminal peptides for profiling of protease substrates Vortragend
Zahedi, Rene P.	Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Deutschland	Temporal quantitative phosphoproteomics of ADP stimulation reveals novel central nodes in platelet activation and inhibition
Zanni, Thomas	Markes International GmbH, Schleussnerstrasse 42, Frankfurt, Germany	FAST MULTIPLEXING OF IONISATION ENERGY FOR PERFORMANCE IMPROVEMENTS IN GC-TOF MS
Zeissig, Sebastian	Center for Regenerative Therapies, Technical University Dresden, Dresden, Germany; Department of Medicine I, University Medical Center Dresden, Technical University Dresden, Dresden, Germany	Lipidomics reveals lipid networks correlated with the progression of human colorectal cancer
Zeller, Martin	Thermo Fisher Scientific, Deutschland	Evaluation of Optimal Conditions for Antibody Subunit Analysis on a Quadrupole-Orbitrap Mass Spectrometer Full Characterization of Antibodies Under Denaturing and Native Conditions on a Hybrid Quadrupole-Orbitrap MS Equipped With a Higher Mass Range
Zhao, Shuang	Department of Chemistry, University of Alberta, Edmonton, Canada	Enabling High-Confidence Human Endogenous Metabolite Identification via High-Resolution MS/MS Retention-Time Library
Zheng, Xueyun	Pacific Northwest National Laboratory, USA	Standardised Collision Cross Section Measurements by Single Static Drift Field Ion Mobility Instrument in an Interlaboratory Study
Zimmermann, Ralf	Helmholtz Zentrum Muenchen, Neuherberg; University of Rostock, Rostock; Universität Rostock, Deutschland	The Usage of Direct Inlet Probe in combination with High Resolution Mass Spectrometry for the Characterization of Heavy Petroleum Products Direct resonance-enhanced multi-photon ionisation (REMPI) of complex liquid samples under vacuum conditions
Zimmermann, Ralf	Joint Mass Spectrometry Centre / Chair of Analytical Chemistry, University of Rostock, 18059 Rostock, Germany; HICE - Helmholtz Virtual of Complex Molecular Systems in Environmental Health – Aerosols and Health, www.hice-vi.eu; Cooperation Group Comprehensive Molecular Analytics, Helmholtz Zentrum München, 85764 Neuherberg, Germany; 2Joint Mass Spectrometry Centre Helmholtz-Zentrum München, Comprehensive Molecular Analytics (CMA), Neuherberg, Germany; Universität Rostock, Deutschland;	Evolved gas analysis ultra high resolution mass spectrometry - Insights into heavy petroleum fractions and combustion aerosol Multiple analysis of individual airborne aerosol particles by laser mass spectrometry: Detection of polyaromatic hydrocarbons from the particle-surface and particle-core Thermal and laser desorption atmospheric pressure photo ionisation ultra high resolution mass spectrometry – Concept and application towards complex samples Thermogravimetry coupled to Ultrafast Gas Chromatography Singlephoton-Ionisation Time-of-Flight-Mass-Spectrometry (TG-SPI-TOF-MS) for Evolved-Gas-Analysis of Fuels regarding to the Deposit Formation Potential

Autor(en)	Organisation(en)	Titel des Beitrags
	Helmholtz-Zentrum München,Deutschland	
Zinn, Nico	Cellzome GmbH, Heidelberg	Analysis of drug-induced effects on proteostasis in cell lines and non-dividing primary cells by quantitative mass spectrometry Vortragend
Zuleger, Nikolaj	MPI of Cell Biology and Genetics, Dresden, Germany	Improved protocol for recovery of vesicular proteins

Integrative Methods for Elucidating the Structure & Function of Cellular Machines

Brian T. Chait
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New York, NY 10065

The myriad events that occur in living cells (replication, organellar assembly, transport, genome organization, transcription etc.) are to a large extent carried out through dynamic associations and assemblies of macromolecules. I will describe our efforts to develop and integrate sets of tools that are designed to throw light on the evolution, structure and function of these macromolecular machines.

At the very earliest stage of analysis, we define the precise ensembles of macromolecular players that make up the assemblies of interest. Mass spectrometry has become an increasingly enabling tool for this task, owing to its sensitivity and its ability to characterize the primary structures of endogenous proteins along with any modifications that may be present. At the next stage of analysis, we apply combined proteomic-biochemical approaches to gain insights into the architectures of protein complexes, especially those that are too large or too poorly behaved for traditional X-ray crystallographic diffraction or NMR spectroscopic analyses. Finally, we integrate data from all these sources to generate models that can provide insights into the evolution, structure and function of these remarkable macromolecular machines. I will to discuss current capabilities and limits of this approach as well as prospects for the future.

Translational mass spectrometry: Molecular images and more.

Ron M.A. Heeren

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New Mass Spectrometry based chemical microscopes that target biomedical tissue analysis in various diseases as well as other chemically complex surfaces have now firmly established themselves in translational research. In concert they elucidate the way in which local environments can influence molecular signaling pathways on various scales, from molecule to man. The integration of this pathway information in a surgical setting is imminent, but innovations that push the boundaries of the technology and its application are still needed. In particular, researchers investigate comprehensive molecular patterns of health and disease. This is a key element needed to pave the way for personalized medicine and tissue regeneration. One barrier to predictive, personalized medicine is the lack of a comprehensive molecular *understanding* at the tissue level. As we grasp the astonishing complexity of biological systems (whether single cells or whole organisms), it becomes more and more evident that within this complexity lies the information needed to provide insight in the origin, progression and treatment of various diseases. The best way to capture disease complexity is to chart and connect multilevel molecular information within a tissue using mass spectrometry and data algorithms. Charting this territory through the generation of molecular atlases from cells and tissue has become reality through the clinical implementation of imaging mass spectrometry complemented with high throughput “omics” approaches. It is evident that a single analytical technology merely yields a subset of the molecular information needed to obtain an in depth understanding of a clinical problem. Multimodal approaches enable the study of clinical samples at a variety of molecular and spatial scales. The distribution of several hundreds of molecules on the surface of complex (biological) surfaces can be determined directly in complementary imaging MS experiment with different desorption and ionization strategies. High throughput, high resolution MALDI techniques offer three dimensional molecular data on the tissue level. The combination with tools from structural biology makes it possible to perform imaging experiments at length scales from cells to patients.

Nucleic acids biophysics: insight from (and into) mass spectrometry

Valérie Gabelica

Inserm, CNRS, Université de Bordeaux, Laboratoire "Acides Nucléiques, Régulations Naturellee et Artificielle" (ARNA, U1212, UMR5320), IECB, Pessac, France; valerie.gabelica@inserm.fr

The general aim of biophysics is to understand the physical and molecular origin of how biomolecules work. Structures tell us how bimolecular systems look like. Thermodynamics tells us why these structures can work in a certain way. Kinetics tells us whether they will work in practice.

Mass spectrometry is a versatile technique to detect, quantify and characterize a wide variety of molecules. Methodological developments to characterize native protein assemblies now give mass spectrometry a place of choice in the field of structural biology. Bridging the gap between structural biology and biophysics then requires to separate coexisting structures, identify and quantify them at equilibrium or as a function of time.

Nucleic acids biophysics—that is the folding, assembly and interaction of nucleic acid structures—is a fascinating subject. A main difference with proteins is that nucleic acids folding is dominated by electrostatic interactions with solvent and counterions, and by hydrogen bonding. As a result, folding landscapes are very rugged and misfolding can prevail. Nucleic acid folding is still difficult to predict, but this is an important subject. Nucleic acid folding regulates gene expression at the transcription or the translational level, and particular folds are attractive targets for drug design.

This motivated our research in developing and exploiting mass spectrometry-based methods to study nucleic acid folding and interactions with small molecule ligands. Along the way, we faced fundamental questions in mass spectrometry (and never took for granted the answers others found for proteins): How does electrospray work? Are all complexes preserved? Do all structures respond equally well? Are the 3D structures preserved? What does collision-induced dissociation tell us about the strength of interactions? Does radical-induced dissociation bring complementary information? How to interpret ion mobility and ion spectroscopy data? These fundamental questions will be illustrated by our studies of duplex and G-quadruplex nucleic acids folding and interaction.

Adventures with Mass Spectrometers: From Designing New Catalysts to Developing a Non-Targeted Drug Metabolite Identification Procedure.

Richard A. J. O'Hair
School of Chemistry, The University of Melbourne
Melbourne, Australia

Modern mass spectrometers are powerful instruments that can either be used as "reactors" to examine the fundamental gas-phase chemistry of reactive intermediates or, when coupled with chromatographic separation techniques, as key analytical discovery tools to explore biological complexity.

In this talk I will discuss recent work aimed at: (1) designing new metal catalysts from the "ground up" [1]; (2) developing a functional model for oxidative damage in DNA [2]; (3) developing an automated and non-targeted procedure for detecting metabolites of drugs, insecticides and known carcinogens without authentic metabolite standards using stable isotope labeling, liquid chromatography mass spectrometry (LCMS), and high performance computing.

References:

[1] Zavras, A. et al., *Nature Communications,* **2016**, *7*, 11746
[2] Feketeová, L. et al., *Phys. Chem. Chem. Phys.*, **2015**, *17*, 258372
[3] Leeming, M. G. et al., *Anal. Chem.*, **2015**, *87*, 4104

Where are ye all? – On the (serious) search for extraterrestrial life

Wolfgang J. Duschl

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Since the 18th century, since the times of Kant and Laplace and their concept of the formation of the solar system, it had been suspected that planets are natural companions of stars, rather than an exception in the case of our Sun. It took, however, until the end of the 20th century to turn this suspicion into an observed fact. In the meantime, we know about around 4000 confirmed planets orbiting stars other than the Sun, and the number is only limited by the time it takes to confirm detections. In the meantime, we started to not only investigate the orbits of these exoplanets, but also their atmospheres. And these investigations will allow us in the near future to search for traces of (simple forms of) life there.

In my talk, I will (1) introduce the methods which are used to identify exoplanets in the first place; (2) discuss the question, in which circumstellar environments we can expect life to exist at all; and (3) present the approaches of how to ultimately identify traces of life in exoplanetary systems.

Multifaceted Shotgun

Andrej Shevchenko

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Shotgun profiling is a powerful analytical tool for rapid, comprehensive and quantitative analysis of complex lipidome. It relies on direct infusion of total lipid extracts from cells, tissues, biofluids and entire model organisms into a high resolution tandem mass spectrometer. Shotgun is an incredibly versatile method which, in rapid succession and with no or minor modifications, could be applied to a variety of biological and biomedical problems from high throughput screening for biomarkers of metabolic disorders to discovery of new lipids in emerging model organisms – all running at the same mass spectrometer, in the same laboratory, using the same software and (almost) the same sample preparation protocol. We envision that shotgun approach could support a concept of the "clonable lab" which implies rapid lateral transfer of methods, standards, skills and software in a form or a single package to any interested laboratory with no previous record in lipidomics.

We will discuss what technological features make shotgun a multifaceted research tool and what limitations they imply. We will also share our experience in applying shotgun lipidomics to human blood plasma screens, diagnostics and treatment of metabolic disorders and understanding the molecular impact of global factors environmental factors e.g. body temperature, diet and development on lipid homeostasis.

Ligand induced oligomerisation of proteins – insights from mass spectrometry

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Introduction

Proteins undergo dynamic interactions with ligands to form catalytic cores, fine-tuned for different cellular action. In some cases, ligand binding induces structural changes of the proteins or promotes the assembly of additional interaction partners. The study of protein-ligand interactions and their resulting complexes is therefore fundamental to the understanding of biological systems. We employed structural mass spectrometry techniques to study (i) binding of autophagy protein Atg18 to the lipid membrane, and (ii) binding of phtalocyanine tetrasulfonate (PcTS) to α-Synuclein – a mediator of neurotransmitter release in nerve terminals. In both cases, ligand binding led to the formation of protein oligomers with known or unknown function. We studied their structures to gain insights into the functional role of these assemblies.

Methods

Proteins were expressed in *E. coli*. Purified proteins were incubated with liposomes (Atg18) or PcTS and protein assemblies were cross-linked with BS3 (bis(sulfosuccinimidyl)suberate) reagent or by photolysis of $[RU(II)bp])_3^{2+}$ (ruthenium(II) tris-bipyridyl dication) in the presence of ammonium persulfate. Cross-linked proteins were (i) digested in solution followed by pre-fractionation of peptides via gel filtration, or (ii) separated by SDS-PAGE and digested in-gel. Generated peptides were analysed by LC-MS/MS on an Orbitrap Fusion Tribrid mass spectrometer (Thermo Scientific). Potential cross-linked di-peptides were identified by database searching employing pLink software. Potential protein-lipid conjugates were identified by database searching using MaxQuant software. Intact protein assemblies were analysed on a Q-ToF Ultima mass spectrometer modified for transmission of high masses.

Results

We used mass spectrometry to study ligand-induced oligomerisation of protein assemblies. We highlight the power of mass spectrometry to study the oligomerisation state as well as the structural arrangements with two examples: (i) autophagy protein Atg18, and (ii) α-Synuclein, which is a mediator of neurotransmission.

Atg18 is a core autophagy protein belonging to the PROPPIN (β-propellers that bind polyphosphoinositides) family. PROPPINs specifically bind phosphatidylinositol-phosphates via two FRRG motifs. We studied Atg18 purified from yeast *Pichia angusta*. We solved the 2.0 Å resolution crystal structure and studied the influence of the FRRG motif on membrane binding. We also used chemical cross-linking and mass spectrometry to study protein interactions in Atg18 in its free or membrane-bound state. We observed intermolecular cross-linked peptides indicating Atg18 oligomerisation in both states. Oligomerisation of Atg18 was confirmed by native mass spectrometry and FRET-based stopped-flow measurements. We further demonstrate that the amine-specific cross-linker Bis(sulfosuccinimidyl)suberate (BS3) which is commonly used for protein-protein cross-linking

can also be applied for cross-linking proteins and phosphatidylethanolamine (PE). Cross-linking experiments with liposome-bound Atg18 thus yielded several PE cross-linked peptides, including two near the FRRG motif.

α-Synuclein is a mediator of neurotransmission in the nerve terminal. It's aggregation considerably contributes to neurodegeneration, e.g. in Parkinson's disease. We found that α–Synuclein can form alpha-helical oligomers through interaction with PcTS - a small molecule. NMR and CD spectroscopy showed that transition to the structured oligomeric state requires the aggregation-prone NAC region of α-Synuclein. Mass spectrometry combined with chemical cross-linking revealed the formation of parallel molecular arrangements in α-Synuclein dimers and tetramers.

These two examples show that mass spectrometry delivers valuable insights into protein oligomerisation. It reveals protein oligomerisation, gives information on the oligomerisation state and uncovers the structural arrangements in the oligomers.

Key words

Cross-linking, oligomerisation, protein interactions, protein-lipid interactions

Temporal quantitative phosphoproteomics of ADP stimulation reveals novel central nodes in platelet activation and inhibition

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Adenosine diphosphate enhances platelet activation by virtually any other stimulant to complete aggregation. It binds specifically to the G-protein–coupled membrane receptors P2Y1 and P2Y12 [1], stimulating intracellular signaling cascades. P2Y12 inhibitors are among the most successful antiplatelet drugs, however, show remarkable variability in efficacy. We applied quantitative temporal phosphoproteomics to study ADP-mediated signaling at unprecedented molecular resolution. We provide temporal profiles of 4797 phosphopeptides, 608 of which showed significant regulation. Our data demonstrate that ADP-triggered phosphorylation occurs predominantly within the first 10 seconds, with many short rather than sustained changes. This study demonstrates an extensive spectrum of human platelet protein phosphorylation in response to ADP and Iloprost, which inversely overlap and represent major activating and inhibitory pathways.

Experimenteller Teil

Fresh blood was obtained from healthy volunteers who had not received any medication for two weeks. Each platelet preparation [2] (biological triplicates) was split into four aliquots. For temporal ADP profiles, aliquots were stimulated with 20 mM of ADP for 10, 30, or 60 seconds, or remained unstimulated. Per donor and experiment, 100 mg of platelet digest were iTRAQ 4plex–labeled, 4 time pointswere pooled, and phosphopeptides were enriched using TiO2 followed by fractionation using hydrophilic interaction liquid chromatography and nano- LC-MS/MS analysis on QExactive. Raw data and Proteome Discoverer results can be accessed via ProteomeXchange (PXD001189).

Ergebnisse und Diskussion

We characterized temporal phosphorylation changes in human platelets stimulated with ADP and ADP Iloprost. Our rationale was that temporal profiles may reveal novel phosphorylation events with important functional roles. Because we aimed to provide an overall picture of the phosphorylation events caused by these major regulators of platelet aggregation, we have chosen to carry out the study under conditions in which the aggregation process is not abolished. Hence, the detected phosphorylation changes will not exclusively comprise initial P2Y1- and P2Y12-mediated events, but also subsequent synergistic effects as a result of integrin outside-in signaling and thromboxane dependent signaling. Although this was not

directly studied, we can confidently assert that the early events with ADP (10 seconds) and Iloprost (30 seconds) are most directly linked to P2Y1, P2Y12, and IP receptor stimulation, respectively. Protein phosphorylation is commonly studied for rather long incubation times and single time points. Thus, reversible events may be overlooked and the detection of early (primary) and late (secondary) events obscured. ADP stimulation induced phosphorylation changes on 302 proteins, for 254 already regulated after 10 seconds. We grouped regulated proteins into four categories: (1) initial processes of activation, (2) aggregation, (3) degranulation, and (4) ubiquitin ligases.

Neue Aspekte

The detection of reciprocal protein phosphorylation may allow the identification of potential marker proteins representing an activation state of platelets.

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Cross-Linking and Mass Spectrometry Shed New Light on the bMunc13-2/Calmodulin Interaction

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Keywords: Calmodulin, Munc13, Cross-Linking, photo-methionine

Introduction

bMunc13-2 is a brain-located isoform of the Munc13 protein family which is essential for the vesicle priming process involved in synaptic short term plasticity[1]. Synaptic vesicle priming is driven by the activation of bMunc13-2 through the highly conserved Ca^{2+}-binding protein calmodulin (CaM), an important signaling protein in various cellular processes. Formation of the complex between bMunc13-2 and CaM induces the assembly of the SNARE complex allowing the synaptic vesicle to fuse with the membrane[2].

Aim of the current study is to gain deeper insights into the bMunc13-2/CaM interaction for a detailed understanding of the priming process. For this, we use cross-linking combined with mass spectrometry, which is an established tool to obtain structural information on proteins and protein-protein complexes[3].

Methods

Recombinant GST-tagged bMunc13-2(367-780) domain and photo-methionine (photo-Met)-labeled CaM were expressed in *E. coli*[4]. Cross-linking experiments were performed with photo-Met-labeled and non-labeled CaM at 25 °C under native-like conditions applying different Ca^{2+} concentrations. In addition to photo-Met, cross-linking reagents with complementary reactivities were employed. MS analysis of cross-linked peptides was performed after digestion with trypsin and GluC followed by nano-HPLC/nano-ESI-MS/MS (Ultimate 3000 RSLC coupled to Orbitrap Fusion Tribrid-MS (Thermo Fisher Scientific)). Data were analyzed with the StavroX and MeroX software tools[5]. Additionally, non-covalent complex formation was investigated by native MS on a high-mass Q-TOF II mass spectrometer (Waters Micromass/MSVision) using 300 mM ammonium acetate. Models of the bMunc13-2/CaM complex were generated by Rosetta.

Results

The use of photo-Met for cross-linking is facile, as the non-directed incorporation of photo-Met into proteins is a straightforward procedure. The translation machinery accepts photo-Met instead of methionine, oblivating the need for additional components, e.g. tRNAs, for the subsequent expression of photo-Met-labeled protein. Photo-Met was successfully incorporated into CaM for subsequent photo-cross-linking experiments, yielding an incorporation rate of >30% [4]. Cross-linking experiments between CaM and the bMunc13-2(367-780) domain relied on the incorporation of photo-Met as well as on a variety of different chemical cross-linkers, revealing an interaction between both proteins. The interaction showed the expected 1:1 stoichiometry between Munc13-2 and CaM, which was confirmed by native MS measurements. Most of the cross-linked amino acids are located in close neighborhood or directly at the proposed CaM binding sites located within the bMunc13-2 domain. For a deeper understanding of the interaction between bMunc13-2 and CaM, a bMunc13-2 (704-742) peptide containing the C-terminal CaM binding site in addition to all identified cross-linked residues flanking this binding site was docked with CaM by Rosetta. The resulting two models show a helical structure of the bMunc13-2 peptide interrupted by a small loop, allowing a slight flexibility at the N-terminus of the peptide. Hence, modeling of the bMunc13-2 peptide/CaM complex revealed new insights into the bMunc13-2/CaM interaction.

New Aspects

Structural investigation of the bMunc13-2/CaM complex by combining the incorporation of photo-methionine and external cross-linkers, MS analysis and computational modeling.

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Abstract title

Metal labelling of tri-functional Capture Compounds (CCs) to detect protein targets of small molecules

Authors

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Introduction

Accurate quantification and identification of proteins and peptides is a challenging element in modern proteomics. Metal tags have been reported as ones that allow to test this aspect. [1] The usage of functionalized small molecule probes to target proteins that specifically bind to drug molecules, followed by detection of lanthanide tags, represents a novel approach in chemical proteomics. Inductively coupled plasma mass spectrometry (ICP-MS) is used for the detection due to its high sensitivity, linearity and matrix robustness.

Experimental section

Tri-functional Capture Compounds (CCs) [2] composed of a selectivity function, a photo-reactive function, and a lanthanide containing detection function were synthesized to detect specifically binding proteins. As a readout, inductively coupled plasma mass spectrometry quantification (ICP-MS) was used. To prove the concept, labelling of an isolated protein and ICP-MS –based quantification was performed, fluorescence detection was used as a reference method. For the further investigations labelling of living cells has been done.

Results and discussion

A first proof of concept experiment was performed on the methyltransferase M. TaqI from *Thermus aquaticus*, showed reproducible labeling (RSD 17%). M. TaqI was targeted by a tri-functional CC containing *S*-adenosyl-L-homocysteine, a product inhibitor of many MTases, as the selectivity function, a photo-reactivity function, and a Tb-DOTA complex as detection function. Gel-based analysis allowed the detection of specific photocross-link of the CC to M. TaqI based on a mass shift of the labeled species, and ICP-MS based quantification allowed an estimation of the cross-link yield of the probe to the target protein. Another CC with the

dopamine D2 receptor (DRD2) antagonist sertindole as selectivity function was used to target DRD2 expressed on the surface of living HEK293 cells. Results are compared to fluorescence readout using ananalogous CC with a fluorescent detection function.

Novel aspects

Application of a tri-functional CC to target specific binders of small molecules, using a metal tag for detection by ICP-MS.

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Keywords

CC - ICP-MS

Neutral loss-triggered EThcD mass spectrometry identifies protein pyrophosphorylation in vivo

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Covalent post-translational modifications (PTMs) modulate the structure and function of proteins.[1]

Protein phosphorylation is one of the most studied PTMs and regulates almost all areas of cell biology, including cell signaling, regulation of enzyme activities, apoptosis and protein-protein interactions. Tandem mass spectrometry (MS/MS) has emerged as the core technology for the reliable identification and localization of new PTMs. Here, we report the mass spectrometric analysis of peptide pyrophosphorylation [2,3], a protein modification that has eluded detection by conventional MS/MS methods.

Experimenteller Teil

Mass spectra were acquired on an Orbitrap Fusion mass spectrometer coupled to a Dionex Ultimate 3000 NCS-3500RS nanoLC. FT survey scans were performed in the range from 350 to 1500 *m/z* at a resolution of 120,000. Precursor ions were isolated with a mass selecting quadrupole and fragmented with a normalized collision energy of 25%. If characteristic neutral losses of 178 and 196 Da were measured an additional EThcD spectra of the same precursor ions was acquired. EThcD spectra were measured in the orbitrap with a resolution of 15,000. Calibrated charge dependent ETD parameters were used for the ETD process and HCD supplemental activation (sa) was enabled. SA collision energy was set according to the charge state of the precursor.

Ergebnisse und Diskussion

The reliable site assignment of di-and multiple phosphorylated peptides by tandem mass spectrometry (MS/MS) constitutes one of the most challenging tasks in MS-based phosphoproteomics. Owing to its sensitivity and speed, collision-induced dissociation (CID) is the most frequently used fragmentation technique for the analysis of phosphoserine (pSer), phosphothreonine (pThr) and phosphotyrosine (pTyr) in peptides. In the present study, we show that pyrophosphopeptides can be distinguished from isobaric diphosphorylated peptides by their characteristic neutral loss pattern generated during reduced collision energy CID. Analysis of site-specifically pyrophosphorylated peptides exhibits [4] a characteristic “triplett” neutral loss pattern of 98, 178 and 196 Da. In addition, we demonstrate that electron-transfer dissociation combined with higher-energy collision dissociation (EThcD) provides outstanding data-rich MS/MS spectra for direct and unambiguous pyrophosphosite assignment. Remarkably, sufficient fragmentation of doubly charged precursors without losing the labile modifications can be achieved by electron-transfer dissociation (ETD) with high supplemental activation, mitigating this classical limitation of ETD. Exploiting the specific CID fragmentation behavior of pyrophosphorylated peptides, we developed a data dependent neutral-loss-triggered (DDNL) EThcD acquisition method. This strategy allows the reliable characterization of *in vitro* pyrophosphorylations and in combination with a selective enrichment procedure [5] unvovered the first pyrophosphorylation sites *in vivo*.

Neue Aspekte

Differentiation of isobaric di-and pyrophosphopeptides using the neutral-loss-pattern, pyrophospho-site assignment via EThcD, first *in vivo* sites

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Title

Analysis of drug-induced effects on proteostasis in cell lines and non-dividing primary cells by quantitative mass spectrometry.

Authors

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Introduction

We have established a mass spectrometric methodology based on pulsed SILAC and chemical labeling to perform multiplexed differential analysis of treatment or stimulation effects on cellular proteostasis. Proteolysis targeting chimeras (PROTACs) are bifunctional molecules linking target proteins to E3-ligases thereby inducing proteasomal degradation of the target protein. The proteostatic effect of a pan-BET bromodomain targeting PROTAC and its differentiation to the originating inhibitor (JQ1) is demonstrated. We further extended the technique to investigate effects on proteostasis in primary non-dividing cell systems exemplified by HSP90 inhibition with 17-AAG in CD4+ T-cells.

Experimental Section

THP-1 cells were grown in heavy SILAC medium (K[$^{13}C_6$ $^{15}N_2$] and R[$^{13}C_6$ $^{15}N_4$]) until complete conversion and subsequently subjected to a pulsed light SILAC medium exchange followed by compound treatment. Sets of inverse experiments were trypsin digested and labeled with TMT reagents.

Primary CD4+ T-cells were kept in light SILAC medium and subsequently subjected to a pulsed SILAC medium exchange followed by compound treatment. A vehicle control is kept in SILAC light and is labeled with formaldehyde (CH_2O) for each donor and used as reference for protein abundance. Pulsed SILAC experiments were labeled with 'heavy' formaldehyde ($^{13}CD_2O$).

Samples were analysed by LC-MS/MS on Q-Exactive + mass spectrometers.

Results and Discussion

Combining pulsed SILAC labeling with isobaric mass tags enabled the comprehensive analysis of effects on proteostatis caused by a PROTAC introduced knock-down of BET bromodomain proteins. Our methodology enables distinguishing PROTAC-induced BET bromodomain degradation events from downstream transcriptional or translational regulation. Reduced abundance in the mature and nascent protein pools of BET family members BRD2, 3, and 4 indicated rapid degradation by the Protac after 6 hours in line with expected trends for direct PROTAC targets. JQ1 alone did not induce effects on mature BET family members while BRD2 new synthesis was increased upon inhibition of BET family members BRD2, 3, and 4.

Since full SILAC conversion of non-dividing primary cells is not feasible we devised an alternative proteomics strategy for investigating drug induced changes in proteostasis by combining pulsed SILAC with reductive dimethylation. This methodology enabled the comprehensive analysis of HSP90

client proteins using the ATP-competitive drug candidate 17-AAG in resting primary CD4+ T-cells derived from two independent donors. In line with the expected mechanism of 17-AAG, HSP90 inhibition is counteracted by an increased new synthesis of heat shock response proteins (HSP1A1, DNAJ11). The glucocorticoide receptor (NR3C1) gathered in an hsp90-/hsp70-based chaperone machinery holding the unliganded receptor in a conformation allowing steroids to access the binding side of the receptor is degraded independently of its maturation state. Additionally, e.g. the receptor tyrosine kinases JAK1 and LCK are prominently reduced in their abundance as mature and nascent proteins indicating a constitutive requirement of these proteins for HSP90. Both proteins are associated with immune response and finally T-cell activation JAK1 in the Jak/Stat Signaling pathway or LCK in the T-cell receptor signaling. We could show that 17-AAG consequently broadly abrogates T-cell activation by anti CD3 and anti CD28.

New Aspects

Pulsed SILAC combined with TMT or reductive dimethylation enables investigation of compound induced effects on proteostasis in cell lines and non-dividing primary cells.

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Keywords

Proteostasis, HSP90, primary cells, PROTAC

Development and implementation of new analytical methods and databases for the detection of additives in fuels and fire debris.

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Modern gasoline and diesel fuels derive a significant part of their performance from the addition of small amounts of chemicals, also referred to as fuel additives [1,2]. The identification of such fuel additives gives a valuable new parameter for forensic fuel identification and sample comparison, especially in complex case situations such as highly burnt samples, as well as additional forensic intelligence by potentially establishing correlations between crime scenes, filling stations and suspects. The chemical structures of such fuel additives are rarely known as they are intellectual properties of the companies and are not identifiable with standard analytical methods for forensic analysis such as gas chromatography-mass spectrometry (GC-MS) due to low concentrations and high molecular structures [3].

To our knowledge, this is one of the first approaches to use fuel additive analysis for forensic applications. New analytical methods for the identification of additives in commercially available gasoline and diesel fuels as well as corresponding databases have been developed to raise the evidential value of forensic investigation in this field. Methods involve simple fuel sample preparation steps and are based on liquid chromatography-mass spectrometry (LC-MS). Separation is achieved on different column materials and various mobile phase systems are applied using gradient elution to optimise the sensitivity of the system. A LTQ XL Orbitrap mass spectrometer fitted with an electrospray (ESI) source and operated in positive ion mode at a scan range between 175-2000 m/z is used for detection.

Various fuel additives and corresponding characteristic polymer distributions are identified with the help of the obtained chromatograms and ion maps to establish differences between fuels of various brands, qualities and areas. Thereby, it becomes evident that the developed method can not only provide brand specific information but can also be used to distinguish fuels from the same brand but of different qualities. Results also imply differences between fuel samples from the same brand and quality but collected at various filling stations within different regions of Germany. MS^n-experiments were performed to identify specific structural elements of substances within a polymer distribution and head groups as well as repetitive units are successfully determined. However, problems occurred as the mass spectrometric method is not yet able to distinguish between branched and unbranched structures. In addition, obtained results are converted into a

database which allows the search of specific monoisotopic masses as well as masses of the corresponding molecular ion of all identified polymer series. Such databases can readily be used for case work and provide additional forensic information of evidential weight but need to be updated constantly.

The newly developed method for fuel additive analysis promises new forensic intelligence and can provide additional information for case work.

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Keywords: *fuel additives, brand recognition, LC-ESI-MS, structure identification, database*

Method development LC-MS, Forensic

Rapid fingerprinting of lignin renewable energy sources by ambient ionization high-resolution mass spectrometry and simplified data mining

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INTRODUCTION

The main goal of valorizing lignin as an efficient and economical source of renewable aromatics is met with the challenge of characterizing and analyzing this vastly diverse heterogeneous aromatic biopolymer. The widely differing sources of lignin (trees, grasses and other vegetation), numerous lignin extraction procedures, chemical modifications and varying depolymerization reactions all add to the complexity of lignin characterization. Lignin structure in itself is fundamentally complex due to the intricate and complex set of linkages, which are the subject of much intense research in elucidating the "lignome"[1]. The work presented here primarily looks at directly screening Kraft alkali lignin employing ambient ionization in developing the first direct analytical method to fingerprint solid lignin samples and advancing simplified data mining.

EXPERIMENTAL

Kraft alkali and Organosolv lignin standards were purchased from Sigma-Aldrich (Steinheim, Germany). Kraft alkali lignin was further subjected to electro-catalytic oxidative cleavage for 24 hours at 180 °C[2]. All ambient ionization (DART, pyrolysis DART and DESI) and ESI sources were coupled with a single stage benchtop Orbitrap high resolution mass spectrometer for full scan high resolution negative ion data collection. All species that were assigned elemental formulae after applying lignin specific data filtering were subjected to data classification approaches based on employing modified Kendrick mass defect filtering[3,4]. Selected modified Kendrick bases were for methoxy [OCH_2] and phenol [C_6H_4O] units and were plotted against DBE values, to separate the detected chemical species based on their degrees of unsaturation and chemical content.

RESULTS

Coupling ambient ionization methods with high resolution mass spectrometry (HRMS) provides enhanced selectivity for rapid broad analyte classifications. This capability was required in this study due to the inherent complexity of the heterogeneous depolymerized lignin samples. DESI was able to provide results over a wider *m/z* range than its plasma-based counterpart, DART, however also ionized more highly saturated compounds with low oxygen to carbon (O/C) ratios and with relatively low double bond equivalents (DBE). The DART direct solid analysis method primarily detected the same core lignin monomeric and dimeric species, as were observed with DESI and ESI, however, a slightly more limited *m/z* range was observed. In contrast to the spray-based methods, the DART spectra were nearly void of the unknown highly saturated compounds demonstrating negative Kendrick mass defects. Plotting modified Kendrick mass defect values against the degree of unsaturation (DBE) firstly permits direct visualization of monomeric, dimeric and trimeric lignin species. Employing methoxy units, [OCH_2] as the Kendrick mass base, lignin compounds differing only by methoxy groups are clustered together and differences based on oxygen and hydrogen content and water loss/addition are clearly observed. To distinctly separate the grouped methoxy-related compounds, a more specific Kendrick base of [C_6H_4O], representing the phenolic lignin core, was applied. The phenolic Kendrick mass defect plotted against DBE yielded broad partitioning of the compounds, while maintaining distinct links and linear associations across monomeric, dimeric and trimeric compounds, as well as among other lignin series, such as bonding types. Pre-filtering the data for lignin characteristic compounds in combination with the novel data mapping principle presented in this work allowed the core lignin compounds to be visually identified. Ambient ionization provided performance much faster than conventional techniques and the novel data mining approach provided rapid global inspection of such complex data sets.

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AP-SMALDI MSI of metabolites and lipids in *Schistosoma mansoni* parasites

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Introduction

According to the World Health Organization (WHO) neglected tropical diseases (NTDs) are an emerging problem, affecting about 1 billion people. Reasons for infection are often a lack of basic sanitation and close contact to infectious vectors. However, new anti-parasite drugs and vaccines are required to prevent such diseases from spreading. Often the metabolome of parasitic vectors is not described nor understood. Mass spectrometry imaging (MSI) is a powerful tool which can be used to visualize such metabolites [1]. Currently we are investigating *Schistosoma mansoni*, a blood fluke causing schistosomiasis (~280 million patients world-wide) in its adult state. It is crucial to characterize the interaction between female and male schistosomes to identify possible novel anti-schistosomal drug targets.

Experimental Section

Adult *S. mansoni* worms were embedded in gelatin and cut into sections using a cryotome. Corresponding worm sections were fixed on a glass slide, and matrix was applied using a home-built pneumatic sprayer. After matrix application, the surface was analyzed via atmospheric pressure (AP) Scanning Microprobe Matrix Assisted Laser Desorption/Ionization (SMALDI) MSI. A lateral resolution of down to 1.4 µm is achievable, using an AP-SMALDI source recently developed by our working group [2]. An orbitrap mass analyzer was used for mass analysis, providing a high mass resolving power and mass accuracy. Data evaluation was performed using software packages MIRION and MSI-Reader and by database assistence.

Results and discussion

Adult schistosomula are 1-5 mm long and 100-350 µm thick. Complete transverse and lengthwise sections of *S. mansoni* males were obtained with 20 µm thicknesses. Due to the structure of adult schistosomes, it is crucial to obtain lengthwise sections of the very few organs such as testes/testes-lobes, esophagus, oral sucker, ventral sucker, gynaecophoric canal where the paring contact between female and male takes place, and tegument, the outer body cover of flatworms.

Worm sections were measured via AP-SMALDI-MSI after spraying 2,5-dihydroxybenzoic acid (positive ionization mode) in a range of *m/z* 250-1000 with a lateral resolution of down to

5 µm per pixel. Several classes of components were detected, mainly lipids and lipid like structures. Lipid classes such as mono-, di- and tri-acylglycerides (MAG, DAG, TAG), phosphatidylethanolamines (PE), phosphatidylinositoles (PI), phosphatidylcholines (PC) and phosphatidylserines (PS) were detected, some of which were identified using e.g. LC-MS [3] (Data evaluation still ongoing). Proposed structures, however, still need to be verified by MS-MS experiments to confirm lipid classes and to assign hydrocarbon chain lengths of fatty acids or ethers, respectively. Several compounds seem to be specific for certain structures e.g. tegument or worm body. By extending the mass range it was also possible to detect possible neuropeptides. Further experiments are required to investigate and verify their amino acid sequence.

Novel aspects

Investigation of the metabolome of adult schistosomula and characterization of male-female interactions during pairing contact on the topographical molecular level.

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Keywords

Mass spectrometry imaging, Atmospheric pressure Matrix Assisted Laser Desorption/Ionization, Schistosomiasis

Effect of ecosystem type and fire on chemistry of WEOM as measured by LDI-TOF-MS and NMR

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Introduction (120 words)

Soil organic matter (SOM) and its water-soluble components play an important role in terrestrial carbon cycling and associated ecosystem functions. Chemically, SOM are complex mixtures of organic compounds derived from decomposing plant material, microbial residues, as well as root exudates, and soil biota. To test the effect of the ecosystem type (forest and grassland) and fires events on the chemistry of dissolved organic matter (DOM), we applied a combination of laser-desorption/ionization time-of-flight mass spectrometry (LDI-TOF-MS) and 2D (^{1}H and ^{13}C) nuclear magnetic resonance (NMR) spectroscopy to water-extractable organic matter (WEOM) from a range of top soil samples. The aim was to assess how suitable LDI-TOF-MS functions for the rapid characterization of WEOM.

Experimental part (120 words)

The soil sampling sites were located in the eastern part of the German Federal State of Thuringia. Two different land use types were selected: grassland and coniferous forest. At each site, fire disturbance was simulated by using a gas powered flame weeder to burn the vegetation by holding it directly onto the ground surface and organic layer, respectively, in a distance of 15 to 20 cm. The top soil material was collected and DOM samples were prepared according to [1] (cold water extracts). Afterwards the solutions were freeze-dried for several days and re-suspended in acetonitrile-d_3/D_2O (70/30, v/v) to perform both analytical techniques LDI-TOF-MS (Bruker UltrafleXtreme) and NMR spectroscopy (Bruker Avance I NMR spectrometer, 400 MHz) on the same samples.

Results and discussion (300 words)

In summary, LDI-TOF-MS and NMR spectroscopy were tested, optimized and successfully employed to shed light on the molecular changes of WEOM induced by ground fires in different ecosystems, forest and grassland sites. The ordination method nonmetric multidimensional scaling (NMDS) analysis was applied to four different LDI-TOF-MS methods (variation of sample concentration, pH value, ion mode, employing the one-factor-at-a-time method). Only one LDI-TOF-MS method enabled the differentiation between fire and non-fire treated samples, as well as between grassland and forest

soils. Furthermore, investigation of the structure-like mass deltas in the average LDI-TOF-MS spectra (n=9) of this method revealed a similar composition of forest and grassland soil, *de facto* polysaccharides and proteins made up the main components, whereas amino-sugars, fatty acids, and sterols only increased as a result of forest burnings in favor of a decrease of the main components. In WEOM from grassland soil, fatty acids and polysaccharides increased as a consequence of fire, explaining for, e.g., the often reported water repellence of burned soils. The additional NMR data highlighted the fire-induced reduction of carbohydrates to a higher extend in forest soil, thus altering the functionality of WEOM. The change in WEOM composition and hence the downward cascading flux of energy and matter may affect other ecosystem processes and functions such the activity of soil microbial communities or the water quality.

Novel aspects (20 words)

LDI-TOF-MS and NMR for exploring the effect of fire on the composition of WEOM in forest and grassland soils.

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Keywords (5)

Water-extractable organic matter, laser-desorption/ionization time-of-flight mass spectrometry, nuclear magnetic resonance spectroscopy, nonmetric multidimensional scaling, fire disturbance

Evolved gas analysis ultra high resolution mass spectrometry - Insights into heavy petroleum fractions and combustion aerosol

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Introduction

The chemical characterisation of heavy petroleum, its fractions as well as combustion aerosol is still a challenging task for analytical chemistry. Mass spectrometry has proven to be an suitable technique for characterising complex mixtures. Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS), with its unbeaten mass accuracy and resolving power, can analyse ultra complex mixtures of thousands of substances and assign elemental compositions. Nonetheless, evolved gas analysis (EGA), a common technique in material characterisation, most often utilizes low resolution mass analyzer. Here we present EGA coupled to ultra high resolution mass spectrometry applying atmospheric pressure ionisation techniques. Several sample sets from the field of Petroleomics as well as combustion aerosol from a ship diesel engine were analyzed.

Experimental

Two approaches were realized: direct thermo desorption atmospheric pressure photo ionisation (APPI), utilizing a home-build source, and hyphenation of a thermo balance to atmospheric pressure chemical ionisation (APCI) [1]. Ultra high resolution mass spectrometry was conducted with a 7 T FT-ICR MS. Besides other a heavy fuel oil fractionation, several heavy crude oils, their Asphaltene fractions (precipitated with different solvents) as well as particulate matter (PM) samples of a ship diesel engine were investigated. The time resolved high resolution mass spectra were pre-processed and exported using the vendor instrument software. Self-build MATLAB algorithms were utilized for defining region of interests. Elemental compositions were assigned to these filtered data within 2 ppm error range and typical restrictions applied in Petroleomics.

Results and Discussion

Both approaches are well suited for the EGA experiments. The time/temperature resolved processing allows the investigation of individual molecular species.

Increasing temperature leads to emission of higher boiling point species. At higher temperatures, pyrolysis changes the pattern. The Asphaltenes showed low signal in the thermo desorption and revealed high aromatic thermal fragments in the pyrolysis step. They emit a complex pattern up to m/z 650. Distinct differences, such as the ratio between the two phases and the elemental composition of the evolved species, were found between the sample types. Furthermore, it was found that the contribution of the desorption phase decreases when applying heavier Alkanes for precipitation.

Interestingly, for the PM the double bond equivalent pattern is rather constant. We address this effect to the dominant emission of higher alkylated species rather than bigger aromatic structures during the direct thermo desorption process.

Additionally to the broadband spectra collision induced dissociation spectra were recorded. The dominant de-alkylation process allows core structure analysis to identify the most important aromatics emitted. The petroleum samples show differences in their CID profile for the different compound classes, e.g. CH-, CHS- and CHN-class species were found in higher abundance, whereas the CHOx-class decline. This finding indicates that nitrogen and sulphur is mainly present in aromatic core structures, whereas oxygen is bound in the side chains.

The results of the CID experiments analysis revealed highly condensed aromatic ring systems. This finding would be an indicator for an higher proportion of the continental-type Asphaltene molecular architecture.

Summarising, EGA coupled to ultra-high resolution mass spectrometry is a promising approach with unique characterisation capabilities for high complex samples, e.g. utilising pyrolysis fragments for structural elucidation of high molecular weight compounds. Furthermore, simulated distillation is feasible and can be characterized on the molecular level. CID gives an additional dimension of characterisation.

New Aspects

Characterisation of evolved gas mixtures emitted by thermal analysis of petroleum and aerosol samples via soft ionisation FT-ICR MS.

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Topics

Instrumentelle Entwicklungen

Umweltanalytik

Keywords

high resolution mass spectrometry, evolved gas analysis,

atmospheric pressure ionisation, petroleomics, combustion aerosol

Proteomic resources for organismal development

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Mass spectrometry based quantitative proteomics has become a powerful tool to compare protein abundance of thousands of proteins in a single experiment. Technically, isotope enriched methods like ICAT, iTRAQ and SILAC can be applied to compare proteomes. However, especially the increased stability of label free quantitation methods in recent years extend the applicability and make it possible to generate large scale proteomic datasets. We employ these improvements to generate large scale resources with a focus on developmental processes.

Experimenteller Teil

Combining stable measurement conditions with pipelined sample preparation and data analysis protocols, we generate time series measurements to follow proteome remodeling during organismal development using a benchtop orbitrap platform. These data are subsequently analysed and made available in interactive R shiny applications to enhance data accessibility for wet lab researchers.

Ergebnisse und Diskussion

We applied quantitative quantitative proteomics to compare two stages of trypanosomes, the procyclic insect form and the bloodstream form of the mammalian host using stable isotope labeling of amino acids (SILAC) to a depth of 4,364 protein groups [1]. Based on this work, we applied label-free quantitative proteomics to investigate the developmental differentiation occurring during these two stages at several time points (long slender, short stumpy, 2h, 4h, 6h, 12h, 24h, 48h and procyclic) in biological quadruplicates also at a depth of 4,270 protein groups [2].

Recently, we focused on *Drosophila melanogaster* and obtained two large scale time series. For the full life cycle with 4-5 conditions per stage (embryo, larvae, pupae and adult), we quantified 7,952 protein groups and noted interesting differences to the formerly generated modENCODE transcriptome. In a second experiment, we obtained a highly time-resolved (measured time points maximal 2 hours apart) embryogenesis dataset for 5,458 protein groups. Both datasets are generated from four independent biological replicates which showcase a very high correlation demonstrating a very high technical reproducibility as well as a very defined biological process. These large scale datasets have been processed using the freely available R shiny applications to produce rich interactive resources for the trypanosome and fly community, respectively.

Neue Aspekte

We apply label-free quantitative proteomics to generate large-scale developmental datasets.

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Direct resonance-enhanced multi-photon ionisation (REMPI) of complex liquid samples under vacuum conditions

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Introduction

Electrospray ionisation (ESI), atmospheric pressure chemical ionisation (APCI) and atmospheric pressure photoionisation/laser ionisation (APPI/APLI) denote the most prevalent soft ionisation techniques for liquid samples. However, the generation of ions from all of these techniques are affected by the sample matrix leading to concurrent ion yields of molecular ions, quasi-molecular ions formed by adducts and fragments. It has been demonstrated that direct electron ionisation (EI) as well as direct and soft single-photon ionisation (SPI) by a VUV lamp is possible for single dissolved compounds, e.g. hexadecane, propofol and eugenol [1]. In this study, we replaced the VUV lamp by an Nd:YAG laser to perform resonance-enhanced multi-photon ionisation (REMPI) [2] at 266 nm for rapid analysis of complex oil samples.

Experimental

The instrumental setup basically consists of a nano-flow UPLC (*nanoAcquity*, Waters Corporation) for sample injection, an Nd.YAG laser (*Minilite I*, Continuum) with 266 nm output and a quadrupole mass spectrometer (*HP5970B*, Hewlett Packard). Six polycyclic aromatic hydrocarbons (PAH), five filtrated (13 mm syringe filter, PTFE (hydrophobic), 0.22 µm) crude oils from different origins and three diesel samples with different contents of biofuel were diluted in dichloromethane and injected by a manual injection valve of 20 nl (VICI AG International) in a continuous solvent flow (400 nl/min) of acetonitrile. Only the tip of the capillary (fused-silica/PEEK, 25 µm ID) is heated to 280°C and ends 1 mm in front of the repeller inside the ion source.

Results & Discussion

After reaching the ion source, the eluents become promptly nebulised followed by desolvation, which is supported by the heater enclosing the repeller. In addition to the original setup, the orifice of the ion source was extended to enable a larger laser spot and consequently higher ion yields.

REMPI under vacuum conditions and moderate light intensities refers to a soft, selective and sensitive ionisation technique for PAHs [2], so molecular ions M^+ of five PAHs were detected from the standard solution while intensities of $[M+1]^+$ fit to the expected isotopic contribution. Moreover, linear correlations between signal intensity and concentration with r^2 of 0.94 or better were obtained.

In the next step, filtrated and diluted crude oils were analysed and compared to REMPI mass spectra of evolved gases released from a thermal balance [3]. Due to simultaneous nebulisation, desolvation and ionisation, the m/z range is extended that compounds which decompose in the thermal balance can be detected. However, homologue series of odd m/z between 200 and 300 dominated the mass spectra of the crude oils which are assigned to ionisation fragments of species with high molecular weight. Those species are considered to have low ionisation energies that the difference to the photon energy becomes larger, leading to their fragmentation. Furthermore, this explanation is supported by the fact that all diesel samples, containing minor amounts of high molecular weight

species, did not reveal homologue series of odd m/z apart from isotopic contribution. Moreover, the addition of 1, 3, 10 and 30% toluene to one crude oil did not affect the mass spectrum except its own molecular ion, proving the independence of the ionisation from the matrix. Finally, a discriminant model for the crude oils was constructed by data projection on predefined vectors [4] to demonstrate the quality of the data for classification.

New Aspects

Rapid screening liquid samples by soft ionisation leading to molecular ions without matrix effects.

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Keywords

photoionisation, crude oil, thermal analysis, evolved gas analysis

Category

Instrumental development

Ionisation techniques

The Aerodynamics of Impactor Spray Ionisation Sources

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Introduction. High flow rate ESI remains the preferred ionisation technique for LC/MS analyses since it offers the most facile coupling for a wide range of analytical flow rates. However, when compared to nanospray ionisation, ESI is known to suffer from poor ionisation efficiency at high flow rates. Here we present a novel impactor spray source which demonstrates significant enhancements in ionisation efficiency when compared to conventional, nebuliser-assisted ESI sources. We will examine the unique aerodynamic features that result from the "cylinder in cross-flow" geometry and give a perspective on how these features may enhance API sensitivity. Particular emphasis will be given to the phenomena of high-We number droplet impacts, the Coanda effect, turbulent vortex shedding and surface microvorticity.

Experimental. Data will be presented that compare the Impactor API source performance with a conventional, nitrogen-assisted ESI source on a triple quadrupole MS instrument. Droplet velocity and size distribution data have been determined using phase Doppler anemometry (PDA) and laser diffraction particle sizing (LDPS) techniques. Data will also be presented from photographic and electron microscopy observations of both the spray dynamics and the impactor surface, respectively. These observations provide direct evidence of Coanda flow, turbulence and microvorticity at the curved surface of the target.

Results and Discussion. A direct comparison of Impactor API versus ESI at flow rates of 0.6mL/min reveal typical Impactor signal enhancements in the range 6.4 - 2.1 for the MRM analysis of verapamil as the mobile phase is varied from 100% aqueous to 100% organic, respectively. From droplet sizing data and PDA velocity measurements, a scheme will be presented that illustrates how the size distribution could be beneficially shifted to smaller diameters by the effect of high Weber number impacts on the hot target surface. Photographic evidence will be presented that shows Coanda streamlines related to the off-axis geometry and the onset of turbulence at the flow separation point. Furthermore, electron micrographs of a used target reveal evidence of counter-rotating microvortices in the region of the flow separation point with a disturbance wavelength of approximately 20µm. It is suggested that this observation shows some correlation with classical cross-flow theory where the wavelength is inversely proportional to the square root of the Reynolds number of the incident gas flow.

Novel aspects. A study of aerodynamic effects which are unique to an Impactor API source.

Keywords. Ionisation, API, electrospray, efficiency, aerodynamics.

Reactive low temperature plasma (LTP) mass spectrometry of neurosteroids

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Introduction

Neurosteroids represent a class of steroids that are synthesized in the brain. They are involved in regulating neurological processes of the brain. Mass spectrometry is one of the key analytical tools for steroid detection and quantification. However, regularly used chromatography-coupled MS methods require many sample preparation steps leading to long analysis times. Ambient ionization techniques, on the other hand, suffer from ion suppression effects and a low ionization efficiency for steroids, hampering sensitive ion detection. To obtain high ionization efficiency while preserving the benefits of ambient ionization, here a reactive low temperature plasma mass spectrometry (LTP-MS) method is introduced for the measurement of neurosteroids. We evaluated the use of this method for the detection of standards, purified extracs, and homogenized mouse brain samples.

Experimental section

A home-built LTP source combined with a linear ion trap / Fourier transform ion cyclotron resonance hybrid mass spectrometer (LTQ FT Ultra, Thermo Fisher Scientific) was used for analysis. Helium served as the main working gas at a flow rate of 500 mL/min. The plasma was generated by dielectric barrier discharge. Standards of the neurosteroids (progesterone, pregnenolone, testosterone, dehydoepiandrosterone, dihydrotestosterone, corticosterone) were dissolved in methanol to prepare solutions of 5 µg/L. Mouse brain was cut longitudinally into two symmetrical parts. Each of the brain tissues was homogenized with ethanol and one of the homogenized samples was prepared following an extraction protocol. The reactive reagent, methylamine was pumped into the gas system at a concentration of 500 ppbv.

Results and discussion

The standard samples of neurosteroids were analyzed using reactive LTP-MS. Methylamine was found to react on the timescale of ionization with steroids containing a carbonyl group. After reactive LTP ionization, steroids were detected as $[M+NH_2CH_3+H]^+$ ions. The protonated methylamine reaction products of neurosteroids showed a 5- to 46-fold increase in peak intensities compared to the $[M+H]^+$ ion signals. The enhanced MS signal intensities suggest that ionization efficiencies of steroids were increased due to the addition of a secondary amino group to the steroid molecules, thereby increasing gas-phase basicity of the modified compounds. Limits of detection (LODs) of the standards were calculated to be as low as ng per mL. This is close to the reported concentrations of steroids present in rodent brains[1]. In addition, steroids extracted from a mouse brain were analyzed. The concentrations of neurosteroids in the brain tissue were calculated through standard addition with formestane as the internal standard. For all the targeted steroids, the calibration plots exhibited good linearity with $R^2 > 0.95$. As a next step towards the

analysis of minimally treated animal tissue sections, LTP-MS measurements of homogenized brain tissue samples without purification or extraction were performed. We were able to detect most ketone-based neurosteroids from mouse brain homogenates. The estimated concentrations of steroids from homogenized samples fell in the same range as those obtained from purified samples. The preliminary results have shown that our reactive LTP-MS workflow allows for rapid and sensitive detection of neurosteroids in brain samples with minimized sample preparation. To further improve our reactive LTP-MS method, the desorption efficiency of the non-volatile steroids needs to be increased. Therefore, we intend to couple our reactive LTP-MS method with other techniques that enhance desorption of sample material.

Novel aspects

A reactive LTP-MS method was developed for sensitive detection of neurosteroids in mouse brain.

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Keywords

Reactive low temperature plasma; ambient mass spectrometry; neurosteroid analysis

Analyse des Peroxid-basierten Sprengstoffs TATP und strukturell verwandter Verbindungen mittels dielektrisch behinderter Entladungsionisations-Massenspektrometrie (DBDI-MS)

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Einleitung

Triacetontriperoxid (TATP) und Diacetonperoxid (DADP) sind peroxidbasierte Initialsprengstoffe, die wegen ihrer Synthese aus einfach verfügbaren Vorläufern vor allem in improvisierten Sprengvorrichtungen Anwendung finden. Ihre hohe Empfindlichkeit gegenüber Stößen, Wärme und Reibung machen ihre Handhabung in größeren Mengen lebensgefährlich. Die Analyse mit klassischen Detektionsmethoden, wie UV/Vis, Fluoreszenz, ESI/APCI-MS und GC-FID/MS ist aufgrund ihrer Struktur und Labilität schwierig. Zur Desorption, Ionisation und Detektion von TATP und DADP von Oberflächen wurde deshalb die dielektrisch behinderte Entladungsionisations-Massenspektrometrie (DBDI-MS), welche auf einem Niedriegtemperaturheliumplasma basiert, eingesetzt.

Experimenteller Teil

Lösungen von TATP und DADP wurden auf verschiedene Oberflächen appliziert und nachfolgend mithilfe der DBDI-MS vermessen. Deuteriertes TATP sowie DADP (TATP-d18, DADP-d12 und DADP-d6) wurden zur Bestätigung der erhaltenen Signale eingesetzt. Zur Quantifizierung von TATP aus Lösungen wurde TATP-3,6,9-13C als interner Stanmdard verwendet. Da aufgrund der Restfeuchte der synthetisierten Peroxide das Einwiegen mit einem großen Fehler verbunden ist, wurde die quantitative Kernspinresonanzspektroskopie (qNMR) zur Bestimmung der Konzentrationen der TATP- und DADP-Lösungen sowie der TATP-3,6,9-13C-Lösung, welche bei der Quantifizierung von TATP mittels DBDI-MS als interner Standard dient, eingesetzt.

Ergebnisse und Diskussion

Bei der Analyse von TATP mittels DBDI-MS weist das Massenspektrum ein Signal bei *m/z* 240 auf, welches dem Ion $[M+NH_4]^+$ entspricht. Die Zuordnung konnte durch die Analyse von deuteriertem TATP (TATP-d_{18}, *m/z* 258) sowie mittels MS/MS-Experimenten bestätigt werden. Im Gegensatz zu TATP wurde DADP als *m/z* 182 detektiert, welches dem Ion $[M+O+NH_4]^+$ entspricht. Messungen von DADP-d_{12} sowie DADP-d_6 bestätigen diese Zuordnung. DADP-d_{12} wird als *m/z* 193 bzw. $[M-D+OH+NH_4]^+$, DADP-d_6 als *m/z* 187 und *m/z* 188, bzw. $[M-D+OH+NH_4]^+$ und

$[M+O+NH_4]^+$, detektiert. Die Detektion von DADP-d_{12} als *m/z* 193 und DADP-d_6 als *m/z* 187 weist auf eine Oxidation von DADP während der Ionisation mittels DBDI hin.

Eine Quantifizierung von TATP konnte mithilfe von TATP-3,6,9-^{13}C als internem Standard erfolgen und mit einer LC/APCI-MS-Methode validiert werden. Mittels der dielektrisch behinderten Entladungsionisations-Massenspektrometrie können peroxidbasierte Sprengstoffen wie TATP, DADP und strukturell verwandte Verbindungen von Oberflächen desorbiert, ionisiert, sowie detektiert und quantifiziert werden.

Neue Aspekte

Anwendung der DBDI-MS zur Detektion und Quantifizierung von TATP sowie DADP von Oberflächen.

Titel

Impact factors on signal response with low temperature plasma ionization for mass spectrometry

Andreas Kiontke[1], Aigerim Galyamova[2], Claudia Birkemeyer[1]

Themen: Ionisationsmethoden
Kategorie: Ambient plasma ionization for mass spectrometry

Einleitung (120 Wörter)

Ambient ionization techniques for mass spectrometry are a rapidly expanding field in analytical research and developed dramatically in the recent past. These techniques perform ionization at atmospheric pressure and enable easy sample preparation, so that analytes can be sampled from their native environment, such as living tissues. Especially the low temperature plasma ionization (LTPI) provides an excellent potential for portability and field-applicability due its possibility for miniaturization based on an easy setup and solvent-free operation. Here, we investigated the relative ionization efficiency of LTPI which depends on instrumental parameters such as electrode geometry or flow rate of the plasma gas and also depends on compound characteristics of analytes and solvents subjected to this ionization.

Experimenteller Teil (120 Wörter)

First, a homemade plasma source was optimized in various ways (type and dimensions of the dielectric, positioning of the electrodes, and type and flow rate of the plasma gas). For the evaluation of the influence of the analyte on the ionization efficiency, a set of 30 anilines was prepared in 50% ACN for each aniline. For assessing the impact of different solvents on the ionization efficiency, a set of six anilines in nine solvents each were measured in three interday replicates. For both analyses the samples were spotted on a paper target and an Esquire 3000+ ion trap mass spectrometer from Bruker equipped with the Data Analysis 3.3 and Esquire Control 5.3 was used.

Ergebnisse und Diskussion (300 Wörter)

After optimization of the plasma source, a signal intensity plateau could be reached with a very low plasma gas flow such as 10 mL/min Helium. This was achieved by 1) reducing the dielectric thickness to a lowest possible value in consideration of the heat arising during operation of the source; 2) minimizing the distance between the electrode and the outlet of the plasma source; 3) shorter distances between plasma source, sample and MS inlet. The responsiveness of 30 anilines was assessed according to the type of the substituent (electron-donating or electron-donating substituents, polar or nonpolar substituents), the position of the substituent, the boiling point, and the analyte's basicity in solution (pKa). In comparison to ESI, the plasma ionization shows a higher selectivity towards the analytes and no dependence on pKa was found. In addition, the behavior of signal response for six anilines in nine common organic solvents each was assessed in dependence on their molecular descriptors, e.g. the boiling point, polarity, solution basicity, and gas phase basicity. Interestingly, we will show that the solvents showed a different tendency to form clusters and

reactions under plasma treatment. Moreover, though an impact of the solvent on the signal response of an analyte is clearly evident, it is outweighed by the influence of the analyte characteristics.

Neue Aspekte (20 Wörter)

We present new insights on the influencing factors of signal response in low temperature plasma ionization for mass spectrometry.

Stichworte: ambient mass spectrometry, aromatic amines, ionization efficiency, low temperature plasma

FAST MULTIPLEXING OF IONISATION ENERGY FOR PERFORMANCE IMPROVEMENTS IN GC-TOF MS

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Time-of-flight mass spectrometry (TOF MS) has made considerable advances in recent years, with the elimination of mass discrimination (crucial for GC couplings), increased sensitivity and compact instrument designs making the technique more amenable. We will explore a number of advances in TOF MS technology which are set to further increase its applicability.

Experimenteller Teil

The term 'multiplexing' is used to describe the combination of multiple data streams into a single, comprehensive stream. Multiplexing can be applied to mass spectrometry in a number of ways but, for the purpose of this presentation, we will focus on fast-switching of electron energies to collect both hard (70 eV) and soft (10-20 eV) electron ionisation spectra within a single run.

Ergebnisse und Diskussion

The novel ion source used in this study enables soft electron ionisation to be performed with no inherent loss in sensitivity. Multiplexing between ionisation energies allows conventional 70 eV spectra to be obtained - for routine identification against commercial libraries - as well as simplified soft EI spectra for enhanced confidence in identification of compounds which may exhibit weak molecular ions and/or similar spectra at 70 eV.

These technological advances will be demonstrated using a number of real-world samples.

Neue Aspekte

Fast multiplexing during acquisition greatly improves the performance of a TOFMS, enabling two complementary MS datasets to be acquired simultaneously.

Titel

Quantitative Positional Isomer Analysis of Mixed Diacyl-Glycerophospholipids (dGPLs) by Ultra Performance Liquid Chromatography-Electrospray-Tandem Mass Spectrometry (UPLC-ESI-MS/MS)

Autoren

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Einleitung

Mixed diacyl-glycerophospholipids (dGPLs) carry two different fatty acids residues abbreviated by A and B that are esterified to glycerol position sn1 and sn2, respectively. Therefore, mixed dGPLs can occur in the two isomeric structures A(sn1)-B(sn2) and B(sn1)-A(sn2). Due to position- and fatty acid-specific action of cellular phospholipid/glycerol acyltransferases, transacylases and lipases, phospholipids of natural origin generally show a typical isomer abundance pattern. Saturated and monounsaturated fatty acids are generally esterified to the sn-1 position, whereas polyunsaturated fatty acids are generally esterified to the sn-2 position of the glycerol backbone (Stern, 1978; Nakanishi, 2010). The alteration of the isomeric pattern, i.e. the relative abundance of dGPL isomers, may be an interesting target for biochemical/biomedical research.

Experimenteller Teil

Reversed-phase UPLC separation using a 30 min gradient (ACQUITY UPLC® CSH™ C18 1.7 µm, 1.0 x 150 mm, Waters) in combination with negative ion mode ESI-MS/MS (Q Exactive™ Hybrid Quadrupole-Orbitrap™, Thermo Scientific) was used as an analytical tool for studying the relative abundances of dGPL isomers. The experiments consisted of mixed full MS and targeted MS/MS experiments with a sampling frequency of about 4 Hz. The setup delivered a set of 100-200 MS/MS scans over a complete UPLC peak. As analytes, standards/lipid mixtures of the glycerophospholipid classes PA, PC, PE, PG, PI and PS purchased from Avanti® Polar Lipids were used as well as bacterial lipid MTBE extracts (Matyash, 2008). Analyses of the UPLC-ESI-MS/MS data sets were performed using the software MassMap®.

Ergebnisse und Diskussion

For a number of fragment ions of dGPL species, different intensities are observed for the pairs of positional isomers. The differences are strongly dependent on the phospholipid class, the fatty acid composition of the individual species as well as the experimental conditions. Since both full MS data and targeted MS/MS data were acquired, the extent of coelution of fragment and molecular ions could be analyzed with a high degree of confidence. Using standard compounds for the GPL classes PA, PC, PE, PG, PI and PS we observed small shifts between the virtually co-eluting ions indicating a marginal separation of acyl positional dGPL isomers by UPLC. The separation is more pronounced in dGPLs consisting of fatty acid residues differing in both acyl chain length and degree of unsaturation. Together

with the intensity differences of the fragment ions of the positional isomers, their partial separation allows for the deconvolution of the peaks of the isomeric forms. The deconvolution is based on the intensity ratios of suitable fragment ions and is done by means of a dedicated module of the software MassMap®. For such calculations, pairs of fatty acid anions as well as any other type of fragment ion pair showing an isomer-specific intensity ratio can be used. Due to generation of isomer-specific elution profiles, the method allows for the determination of relative positional isomer abundances in isomer mixtures. The approach is highly sensitive and can be applied to synthetic mixed dGPL standards as well as to mixed dGPL species of biological origin. With given isomer-specific fragment ion ratios, the relative abundance of individual dGPL isomers can be derived for basically every GPL class.

Neue Aspekte

Fragment ion intensity ratio profiles in UPLC-MS/MS as quantitative probe for the isomeric composition of mixed diacyl-glycerophospholipids.

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Stichworte:

UPLC-MS/MS of phospholipid positional isomers, positional analysis of fatty acids, mixed diacyl-glycerophospholipids, structure analysis of glycerophospholipids, quantitative fragment ion analysis

Themengebiete:

LC-MS, Lipidanalytik/Lipidomics

Fragmentation behavior of neuronal lipids by HCD-MS/MS

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Biological membranes provide hydrophobic barriers to separate the interior of cells and cellular compartments from their outer environment. The transport of material and information through the membranes is usually carried out by the proteins that reside in the membranes. Transfer of information can also be accomplished by membrane fusion, e.g. in neuronal synapses during neurotransmitter release. This process is triggered by membrane proteins and their interplay with specific lipids. However, the role of the lipids in these processes is poorly understood and a complete description of the membranes is therefore of fundamental importance. We studied the fragmentation of neuronal lipids by mass spectrometry to establish a reliable workflow for lipid identification and quantification in complex mixtures such as neuronal membranes.

Lipid standards representing various neuronal membrane lipid classes were purchased form Avanti Polar Lipids. These included Phosphatidylglycerols (PG), Phosphatidylethanolamines (PE), Phosphatidylcholines (PC), Phosphatidylserines (PS), Phosphatidylinositols (PI) and Sphingomyelin (SM). We employed high energy collisional dissociation (HCD) tandem mass spectrometry on a Q Exactive Plus Hybrid Quadrupole-Orbitrap mass spectrometer (Thermo Fisher) to study their fragmentation behavior. High resolution fragment spectra were acquired using an energy ramp in 2 eV increments during direct infusion of the lipid standards. Lipid structures were characterized by means of different energies and polarities producing diagnostic fragment ions. Lipid isomers were quantified relatively by calculating their theoretical isotope patterns and simulating overlapping peak envelopes.

Our aim was the identification of lipids and the determination of their isomers in direct infusion experiments. Structure assignment by fragmentation proved reliable for mixtures even without chromatographic separation. We characterized HCD energy levels in both ion modes likely providing diagnostic fragments for the main neuronal lipid classes and obtained information on the quantitative distribution of lipid isomers.
In negative mode, head group associated ions reached highest intensities at around -16 eV for PE, PS, PI, PG and SM. Similarly, positive polarity contributed mainly to head group identification. Exceptions are PG and PC for which no diagnostic head group fragments were observed in positive mode. Acyl chain fragments reached top intensities at around -35 eV indicating higher stability for the esters bonds. Full acyl chain identification was possible in negative mode for most lipids. SM, however, showed all characteristic fragment ions in positive but not in negative ion mode. PE differed from other lipids by its high stability; loss of the PE head group required twice the fragmentation energy. Similarly, acyl chains of PEs appear to be stabilized after loss of the first chain resulting in higher energies needed for loss of the second acyl chain. PC acyl side chains were not observed over a broad energy range and needed a significantly higher energy to induce their dissociation (approx. 40 eV instead of approx. 30 eV as observed for other lipids).
Relative quantification by isotopic cluster simulation further enabled identification of lipid isomers, e.g. for an SM cluster observed between m/z 729.6 and 735.6 we could determine the proportion of SM(34:0) to be 7%, of SM(34:1) to be 83% and of SM(34:2) to be 9%,respectively.
We are positive that our fragmentation analysis of specific lipids will aid global analysis of natural neuronal membranes in future studies.

Novel Aspects:

Fragmentation characteristics and relative quantification of neuronal lipids in mixtures.

oxLipidomics data integration for systems medicine view on metabolic diseases

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Many human diseases, including obesity, diabetes and atherosclerosis, are accompanied by chronic inflammation and closely connected to oxidative stress (OS). OS can oxidize virtually all biomolecules of which lipids represent one of the most prominent targets. Lipid peroxidation products (LPPs) are chemically diverse group of biomolecules with a variety of functional activities. Many LPPs were shown to play an important role in the onset and development of OS-related diseases and can serve as diagnostic and prognostic biomarkers. However, to include LPPs in a systems medicine view on disease pathogenesis the information on their structures, activities and functions as well as associations with various pathological conditions need to be collected and summarized.

Experimenteller Teil

To address the variety of LPPs in biological samples we developed LC-MS based oxLipidomics analytical platform which allows us to target up to six different LPP classes (oxidized, nitrated fatty acids, oxysterols, electrophilic aldehydes, head group modified and oxidized PLs). To facilitate high-throughput workflows several software tools were developed for lipid (LipidHunter) and LPP (TheoLPP) identification. Finally, experimental and publically available information on oxidized lipids is integrated via knowledge based database LPPdb.

Ergebnisse und Diskussion

oxLipidomics platform was cross-validated using cellular models of oxidative stress (e.g. primary cardiomyocytes) and clinical samples (blood plasma and adipose tissue) from patients with obesity and type II diabetes. The overall analytical solution for LPPs analysis includes optimized reverse phase chromatography protocols combined with targeted (multiple reaction monitoring) and untargeted (data-dependent and independent acquisition) MS techniques [1-5]. New software LipidHunter was developed and validated for high-throughput confident identification of phospho- and glycerolipids. Additionally, a combination of spectral libraries and theoretical fragmentation approaches allowed accurate identification and quantification of oxidized lipids in complex biological samples using in-house developed TheoLPP tool.

To facilitate data management and integrate our experimental information with publically available data on LPPs, a first database aiming to accumulate current knowledge on oxidized lipids, structure the information, and provide the community with a resource useful for researchers from chemistry, biology, medicine, and clinics was introduced. LPPdb will provide a platform to scientists from academia, clinics and industry to support the identification of different LPP species form high-throughput lipidomics for biomarker discovery and validation and thus help to determine "biomarker signatures" to assess pathological processes.

Neue Aspekte

New analytical and bioinformatics platform to facilitate systems wide application of oxLipidomics in metabolic diseases research

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Charge Switching of Phospholipids using Paternó-Büchi Reactions

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Keywords: Lipidomics, Paternó-Büchi Reaction, Charge Switching

Introduction (120)

Mass spectrometric detection of certain lipid classes still remains challenging. For example, protonation barely occurs for analytes that lack basic sites or functional groups, i.e. acidic lipids are difficult to detect in positive ion mode. This has resulted in lengthy sample preparation for HPLC or shotgun experiments, and specific experimental workflows for every lipid class are often required. This particularly concerns phosphatidylinositols and free fatty acids. To bypass this problem, we combined nano-electrospray ionization with a Paternó-Büchi (PB) reaction scheme.[1,2] This photochemical addition reaction is driven by UV-light, forming an oxetane from a carbonyl and an olefinic double bond. By adding a basic group to the carbonyl, we were able to detect acidic unsaturated lipids in positive ion mode.

Method (120)

Charge switching experiments were performed by preparing solutions containing the desired lipid (1 mmol L^{-1}) in a 1:1 mixture of methanol and 2-, 3- or 4- acetylpyridine. Formic acid was added until pH < 7 and the solution was transferred into a gold-coated emitter tip with an inner diameter of 5 µm (DNU-MS). A voltage of 1,5 kV was applied between the nano spray tips and the MS inlet. During ionization the nano-spray tip was illuminated by a commercial handheld mercury UV-lamp (UVP) with an emission maximum at 254 nm, placed inside the ion source in close proximity to the emitter tip. Mass spectra were recorded with a linear ion trap mass spectrometer (LTQ, Thermo Fisher Scientific).

Results (300)

In order to develop a workflow and optimize the new PB method, mass spectra of unsaturated fatty acid standards and methyl esters were recorded in positive ion mode performing PB charge switching experiments. Upon illumination with light of 254 nm, reaction products 121 Da above the corresponding protonated analyte signals were detected, indicating the formation of $[M+acetylpyridine+H]^+$. The maximum PB reaction yield after 2 minutes of UV irradiation resulted in a 5- to 75-fold improvement of the PB reaction product ion intensity compared to the corresponding protonated analyte molecules. Collision-induced dissociation (CID) of $[M+acetylpyridine+H]^+$ was expected to cleave the lipid's oxetane giving rise to two specific fragments. Surprisingly, fragmentation of the PB product of 2-acetylpyridine primarily led to the loss of water from the molecule, whereas fragmentation of the photoproducts from 3- and 4-acetylpyridine indicated cleavage of the oxetane. This result is consistent with a hydrogen bond directed PB reactivity that depends on the position of the carbonyl group on the pyridine ring.[3] The sensitivity increase due to charge switching and the CID efficiency with regard to obtaining double bond specific fragments were most beneficial for the case of 3-acetylpyridine, which was chosen as PB reagent for further experiments. As a next step, the developed PB workflow was used to charge-switch phosphatidylinositol (PI) standards. The PB reaction allowed detecting PIs in positive ion mode and determining double bond positions in fatty acid side chains. The workflow was used to study free fatty acids and PIs in lipid extracts of mouse organs in positive ion mode. Sensitivity increase and double bond specificity allowed assigning several free fatty acids and PIs. The developed workflow will be employed for shotgun lipidomic studies and post-HPLC functionalization experiments of complex biological samples in the future.

Acknowledgement

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New Aspects (20)

Detection of unsaturated apolar and acidic lipids in positive ion mode with improved sensitivity and distinguishing corresponding double bond isomers.

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Software platform to improve the quality control of Lipid mediator quantification

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Introduction:

Lipid mediators (LMs) are bioactive derivatives of ω-3 and ω-6 polyunsaturated fatty acids (PUFA). The identification and quantification of PUFAs and their derivatives by LC-MS^2 enables a comprehensive insight into the regulation of immune cell activities. Generally, QqQ-MS with only unit resolution are applied to study LM metabolism focusing exclusively on selected fragments that are recorded using multiple reaction monitoring (MRM). In contrast, we recorded the complete fragmentation pattern using QExactive and Q-TOF instruments. We studied the improvements in specificity and evaluated the quantification abilities using high resolution MS. A software tool was developed to manage spectral libraries and perform spectral scoring for LM analysis. We tested the software in LC-MS^2 analyses in an infection model of *M. tuberculosis.*

Experimental design:

A set of 52 reference compounds were analyzed on the QExactive Plus (Thermo Fisher Scientific) together with a set of 36 reference compounds on the Q-TOF (Waters). Each compound were dissolved at a concentration of 250 fmol/µl in Solvent A, a mixture of Water/ACN/10mM ammonium acetate/ Acetic acid (59+40+1+0.05;v/v/v/v) and was analyzed by direct infusion (DI) experiments. The averaged MS^2 spectrum was computed from 0.5 min acquisition time and three technical replicates were recorded. The LC-MS was performed using a 1100 micro-LC system (Agilent Technologies) and a QExcative Plus using a Luna C18 (2) column (0.3 mm ID x 150 mm, Phenomenex). Quantification was performed with Xcalibur software (Thermo Fisher Scientific) and MassLynxTM 4.0. (Waters).

Results and Discussion:

In this study, we analyzed the full MS^2 spectra of reference compounds for pairwise spectrum-spectrum matches to develop a spectral comparison score (SCS). The SCS is based on Spearman's rank correlation of relative intensities of matched fragment signals. A software platform was developed that allows to 1) process raw peak lists, 2) generate customized spectral libraries, 3) perform spectral comparisons and 4) helps to identify quantifier ions. Additionally a filter was incorporated that ensures that only fragments with the compositional constraint of $C_nH_{3/2n-y}O_z$ (n=4,5,6…22; y: 0,1,2;

z=0,1,2..5) are considered. During evaluation of the spectra library, even numbered m/z values were detected for some isomers, which are not expected for the given sum composition constraint. Examination using different MS devices (LTQ-Orbitrap, LTQ, Q-TOF, QExactive) make it plausible that radical species are formed and can help to improve the identification of 12-HETE, 11,12-EET, 7-Mar1 and PD1.

First, we tested the tool with spectral libraries of reference compounds. For that spectral information of 52 reference compounds were recorded on the QExactive Puls and for 36 on the Q-TOF, respectively. We calculated all forward and backward spectrum-spectrum matches (SSM) for the LMs acquired on the Qq-TOF and the QExactive Plus, respectively.
In general, the algorithm was capable to score LM in correlation to the structural similarity. The determined false discovery rates indicated that the approach is a suitable quality control. However, a clear cut improvement in the specificity could be determined for high resolution mass spectrometry since mass differences of 0.036 Da, which are characteristic for the exchange of an oxygen with CH_4, were detectable. In this content we could show that known quantifier ions are in many cases not specific for one LM.

Finally, we applied the software for the evaluation of LMs quantitation in an infection model of *M. tuberculosis*.

New Aspect

A new software platform was developed to improve quality control for lipid mediator identification and quantification.

Keywords

Lipid mediators, Spectra comparison score, HR-MS, quality control

Topic: Lipid mediators and Lipidomics

ID: 206 / MoV_1b: 3
Vortrag
Themen: Lipide & Lipidomics
Stichworte: lipidomics, colorectal cancer

Lipidomics reveals lipid networks correlated with the progression of human colorectal cancer

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Colorectal cancer (CRC) is one of the most common and deadly cancers in the world. It originates from epithelial cells lining the colon or the rectum when balance between cell death and proliferation is perturbed. The tumors could infiltrate intestinal wall to invade nearby tissues, spread to lymph nodes, and metastasize to other organs - these features determine pathologic stages of CRC. Colorectal tumorigenesis has long been associated with the perturbed lipid metabolism, however, a systematic lipidomic study is still lacking.

Experimenteller Teil

We conducted a study on a cohort of 20 CRC patients with matched age, gender and body mass index. Both colorectal tumors and peripheral healthy colonic tissues were collected in surgery from each patient and the pathologic stage was determined. Lipids were extracted by methyl-tert-butyl ether (MTBE) and a shotgun lipidomic analysis was performed on a Q Exactive instrument equipped with a robotic nanoflow ion source TriVersa NanoMate using nanoelectrospray chips. Lipids were identified by LipidXplorer software and in total 398 molecular species from 20 major lipid classes were quantified[1].

Ergebnisse und Diskussion

We observed that several lipid classes were significantly changed in colorectal tumors compared with healthy tissues, and we established an interaction network of individual species that are correlated with tumorigenesis[2]. Moreover, we examined the association between tumor lipidomes and different stages in CRC. Lipid species contributing to the progression of CRC were identified.

Our study for the first time comprehensively characterized lipid changes in colorectal tumors and identified lipids responsible for the advancement of CRC. These results would benefit biological functional studies and may confer new insights into the mechanisms of CRC pathophysiology.

Neue Aspekte

Our results correlate lipid perturbation with the progressive tumorigenesis in human colon.

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Development of an advanced nano-LC/NSI method of global lipidomics

Introduction

Lipids are key players of cellular systems that are particularly known for their roles in structural compartmentalization and energy storage. Furthermore, they are also able to fulfill signaling functions in biological systems at marginal concentrations. In order to identify low abundant lipids such as mediators, analytical methods need to be developed that allow an accurate characterization and quantification of these biomolecules with high sensitivity and specificity. In comparison to conventional LC/ESI MS analyses, nano-LC/NSI MS systems promise significant higher measurement sensitivity, reduced sample consumption, and decreased solvent usage. However, such nano approaches have not been widely applied for global lipidomics so far.

Experimental

A nano-LC/NSI MS method for global lipidomics was developed that utilizes an UltiMate™ 3000RSLCnano System (ThermoFisher Scientific) for HPLC separations on a 300 mm x 100 µm self-packed capillary column (column material: Ascentis® Express C18 with 2.7 µm Fused-Core® particles). Lipid detection was performed using a Q Exactive™ Plus (ThermoFisher Scientific) applying parallel reaction monitoring (PRM). The developed nano-LC/NSI MS approach was benchmarked in terms of sensitivity to a narrow bore system (150 mm x 2.1 mm, Ascentis® Express C18 with 2.7 µm Fused-Core® particles) using comparable chromatographic conditions.

Results and Discussion

We developed a nano-LC/NSI MS method that allows analysis of both weak hydrophobic lipids, such as lysophospholipids or sphingosines, and hydrophobic lipids such as triglycerides and cholesterol esters in a single chromatographic separation. In this regard, we optimized the injection procedures into the system to guarantee an uncompromised analysis of both weak hydrophobic and hydrophobic analytes. We also improved detection sensitivity and peak shape of lipids that carry free phosphate groups (e.g. PA, CerP, S1P) by optimization of the solvent compositions.

The reproducibility of the developed method was shown through 25 repetitive separations of a yeast extract that was spiked with lipids standards of 21 lipid classes. Furthermore, the lipid detection sensitivity of the nano-LC/NSI MS system was benchmarked to the corresponding narrow-bore LC/ESI MS system. For all lipid classes, the nano-LC/NSI system was found to be more sensitive than the corresponding narrow-bore LC system. Linear ranges of up to 4 orders of magnitude and LOQs in the attomolar range within the yeast lipid matrix were achieved.

Novel Aspects

Here we established a reproducible nano-LC-NSI MS method that displays an unmet sensitivity and dynamic range for lipid analysis.

Abstract DGMS, Kiel, 2017

Differentiating wild and mutant *C. elegans* using high-resolution atmospheric pressure matrix assisted laser desorption/ionization mass spectrometry imaging

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Introduction

C. elegans (Caenorhabditis elegans) is an important genetic model organism that was first employed to understand the development of the nervous system. Meanwhile it has proven very useful in understanding development, ageing, programmed cell death, etc. Lipid metabolism plays a central role in the regulation of many of these processes but very little is known about the precise localization of lipid molecules within the worm. We set out to measure specific lipid molecules and their precise localization within the worm by using mass spectrometry imaging (MSI). Besides developing dedicated sample preparation methods, we successfully integrated whole body MSI in genetics workflows through the comparison of wild type (N2 Bristol strain) with hyl-1, hyl-2 and lagr-1 ceramide synthase mutants of *C. elegans*.

Method

Worms were washed with M9 buffer, anesthetized with toxic sodium azide in M9, washed with 10 mmol/L ammonium acetate (pH6.5) and transferred gently onto Superfrost/Plus slides for MSI analysis. Samples were stored at -26 °C until matrix application. All imaging experiments were accomplished by using an atmospheric pressure scanning microprobe matrix assisted laser desorption/ionization imaging ion source (AP-SMALDI10®, TransMIT GmbH, Giessen, Germany), coupled to a Fourier transform orbital trapping mass spectrometer (Q Exactive™, Thermo Fisher Scientific GmbH, Bremen, Germany). For soft ionization, organic matrix compounds such as 2,5

dihydroxybenzoic acid (DHB) or α-Cyano-4-hydroxycinnamic acid (CHCA) were homogeneously deposited as an ultrafine spray by using a dedicated matrix preparation unit ("SMALDI Prep", TransMIT GmbH, Giessen, Germany).

Results

We detected significant differences in several sphingolipid compounds such as sphingomyelin (SM) on genetically modified ceramide synthase (Cer-synthase) nematodes compared to wild types. Cer-synthase mutants show a clear increase in several SM signals compared to wild types in the tip of the head. This is the location where the cuticle that covers most of the animal's surface has openings to expose several sensory neurons in the sensilla of the lip region around the mouth of nematodes. Sphingomyelin is a typical neuronal lipid, and high resolution MALDI imaging is able to probe the lipid composition of these neurons. Our instrumentation provided high mass resolution and mass accuracy, combined with on-tissue MS/MS acquisition, providing precise differentiation of particular neuronal sphingolipids from worm surfaces based on high spatial resolution (5µm/pixel) and mass accuracy within ±5 ppm. By using DHB and CHCA as a matrix for soft ionization, our approach allowed the identification and differentiation of protonated, sodiated and potassiated lipid species at high detection sensitivity in positive ion mode imaging studies. We believe that this technique provides great potential in the metabolomics analysis of nematodes, based on the high lateral resolution of the method.

New Aspects:

High resolution AP-SMALDI MSI of adult nematode external cuticular surface to visualize and differentiate biomolecules based on high spatial resolution and mass accuracy

Keywords*:*

High resolution AP-SMALDI imaging, nematodes, *Caenorhabditis elegans*, neuronal lipids, sensory neurons

Bioimaging of photosensitizers in human brain tumors after fluorescence-guided resection

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Introduction

Glioblastoma is the most common malignant brain tumor. An extensive resection of malignant glioma cells can significantly improve the survival rate of the patients. In a fluorescent-guided surgery (FGS), resection is supported by contrast enhancement using a fluorescent dye. The major proagent for FGS is 5-aminolevulinic acid (5-ALA), a natural biochemical precursor of heme b, with fluorescent protoporphyrin IX (PPIX) as intermediate product. After oral administration of 5-ALA, it is transported through the disrupted blood-brain barrier into tumor tissue. Based on the fluorescence of formed PPIX, tumor tissue can be differentiated from healthy brain tissue. In this study, the complementary use of molecular and elemental imaging is presented to examine possible limitations by false positive and false negative fluorescence.

Methods

After resection of the human cerebral tumor, 10 µm cryosections were prepared. The distribution of 5-ALA, PPIX and heme b in the tumor tissue was investigated by matrix-assisted laser desorption/ionization-mass spectrometry (MALDI-MS) imaging. Four positive ion mode experiments in MS and MS/MS mode were performed using a focal laser spot of 20-25 µm and a step size of 50 µm. The matrix α-cyano-4-hydroxycinnamic acid (CHCA) was sublimated and recrystallized before analysis.

The Fe distribution was examined by laser ablation-inductively coupled plasma-mass spectrometry (LA-ICP-MS). Cryosections were ablated linewise with a 50 µm spot diameter and 100 µm/s scan speed using a low volume custom-built ablation cell with a laminar gas flow. Quantitative data were obtained by external calibration with matrix-matched standards.

Results

The developed MALDI-MS and MALDI-MS/MS imaging method was applied to several human brain tumors with different tissue characteristics. MALDI-MS analysis was used to examine and correlate the distribution of 5-ALA, PPIX and heme b. Moreover, the performance of MALDI-MS/MS imaging experiments in case of PPIX and heme b could improve limits of detection and validate MS data. In case of glioblastoma, an inverse correlation of 5-ALA and PPIX distribution was observed with an increased PPIX accumulation in areas of high tumor cell density. Heme b accumulation correlated with blood vessel distribution and areas of hemorrhage. In necrotic tissue, neither 5-ALA nor PPIX were detected, which is in accordance with the absence of fluorescence during FGS. Furthermore, a gliosarcoma, one rare type of glioma appearing non-fluorescent during FGS, was investigated. An explanation for this limited fluorescence has not yet been reported. MALDI-MS(/MS) revealed the penetration of 5-ALA into gliosarcoma tissue whereas PPIX was not detected indicating an impaired PPIX formation. Spatially resolved molecular analysis was complemented by quantitative elemental bioimaging of Fe using LA-ICP-MS. Fe accumulations up to 200 µg/g could be detected in the tumor tissue correlating well with heme b and blood vessel distribution.

Novel aspects

Investigation of human brain tumors after fluorescence-guided resection by the complementary use of MALDI-MS(/MS) and LA-ICP-MS imaging.

Imaging of Cerium Oxide Nanoparticles and Phospholipids in Rat Lung Tissue by Means of LA-ICP-MS and MALDI-MS

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Introduction

Cerium oxide nanoparticles (NP) can be found in a wide range of applications, for example in solar cells and catalysis, such as diesel fuel catalyst to enhance combustion efficiency. The uptake of air-borne cerium oxide NPs from diesel exhaust via inhalation may pose a health hazard for humans. As cerium oxide NP elicit lung inflammation and fibrosis, knowledge about both, its distribution in the lung and its biologic effects is needed to unravel potential mechanisms of toxicity. Here we combined the imaging techniques laser ablation-inductively coupled plasma-mass spectrometry (LA-ICP-MS) and matrix-assisted laser desorption/ionization-MS (MALDI-MS) to study the distribution of cerium oxide NP in the lung along with associated changes of phospholipid distribution.

Experimental part

Cerium oxide NP were intratracheally instilled into rat lungs and cryo-sections were prepared from the cryomatrix-filled lung 3 and 90 days post application. For LA-ICP-MS analysis sections were fixed with formalin, washed and dried. Ablation was performed line-by-line with a 213 nm Nd:YAG laser and 50 µm spot size. Quantification was carried out with standards based on gelatin, containing different concentrations of cerium. The external calibration showed a good linear correlation in the range from 1 to 5000 µg/g cerium. For MALDI-MS the cryo-matrix was removed from lung sections with cold 50 mM ammonium acetate. Dihydroxybenzoic acid and 9-aminoacridine were used for the positive and negative mode, respectively. Phospholipids were identified via exact masses and fragmentation experiments.

Results and Discussion

By LA-ICP-MS, cerium was detected throughout the lung parenchyma. Overall concentrations depended on the instilled concentrations of nanoparticles, which ranged from 0.6 to 4.8 mg per lung. Maximum values could exceed 5000 µg/g. Interestingly, the cerium distribution changed over time and changed from an even to a more concentrated distribution pattern, suggesting progressive compartmentalization. By recording additional naturally occurring elements like phosphorus, the cerium signals could be correlated to biological structures. Alterations of the phosphorus distribution were especially pronounced upon high doses and after longer incubation times. Most striking, cerium deposits were often surrounded by zones with high phosphorus, suggesting a correlation between cerium deposition and tissue alteration.

MALDI-MS experiments confirmed that zones with increased phosphorus concentration were due, at least in part, to elevated levels to phospholipids. This is in good accordance to previous studies in the literature, that found an increased phospholipid content in bronchoalveolar lavage fluid of rat lungs

treated with cerium oxide.[1] Here, the additional MALDI-MS imaging revealed a hitherto unexplained variety in the distribution of different phospholipids. For example, there was a significant zonal difference in the distribution pattern of PC 32:0, which is the most abundant phospholipid in lung surfactant, and its monounsaturated form PC 32:1. In order to identify the phospholipids, fragmentation experiments were carried out. Via characteristic fragments, for example *m/z* 184.074 for phosphatidylcholines, an accurate classification was achieved.

The study shows that combining different elemental and molecular imaging techniques allows to link up primary and secondary distribution of nanoparticles in lung sections with characteristic alterations of phospholipids, whose biologic significance remains to be determined.

New aspects

Direct correlation between NP and alterations in the tissue is demonstrated by applying elemental and molecular imaging techniques.

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Keywords

LA-ICP-MS, MALDI-MS, imaging, Nanoparticles

Implementation of a High Repetition-Rate Laser System in an AP-SMALDI MSI System for Enhanced Measurement Speed

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Keywords: Instrumentation, Imaging, MALDI

Introduction (100)

Mass spectrometry imaging (MSI), especially under atmospheric pressure (AP) has seen rapid growth of interest in chemistry, biology and medicine.[1] Owing to its high sensitivity and high lateral resolution of better than 10 µm, matrix-assisted laser desorption/ionization (MALDI) MSI has become a powerful technique for analyzing surfaces and tissue sections. In recent years, considerable efforts have improved lateral resolution, analytical sensitivity and acquisition speed.[2–4] Implementation of a high repetition-rate laser systems in an AP MALDI MSI source allows mass spectrometry imaging of larger tissue areas and enables high throughput applications in a continuous raster mode.

Method (130)

MALDI MSI was performed using a home-built atmospheric-pressure imaging ion source coupled to an orbital trapping mass spectrometer (Q Exactive HF, Thermo Fisher Scientific GmbH, Bremen). The MALDI MSI experimental setup is based on an AP-SMALDI10® MSI source (TransMIT GmbH, Giessen), but employs a high repetition rate diode-pumped solid-state laser system generating 343 nm laser light with up to 2 kHz repetition rate (FLARE NX 343-0.2-2, Coherent GmbH). DHB or CHCA matrix solution was sprayed onto the tissue section surface using a SMALDIPrep (TransMIT GmbH) ultrafine pneumatic sprayer system. The laser and the MSI source were controlled by a home-built MATLAB (R2016a, The MathWorks GmbH) control program.

Results (250)

A high repetition rate laser system was implemented in an AP-SMALDI10 MSI system in order to enhance the measurement speed and to study fundamentals of the MALDI process. The diode-pumped solid-state (DPSS) laser system (Yb:YAG) generates frequency tripled laser light with 343 nm wavelength, pulse durations of ~1 ns and repetition rates up to 2 kHz. The influence of the laser pulse repetition rate on the ablation/desorption behavior and on mass spectral quality were studied. Experiments were performed on dried-droplet and matrix spray-coated mouse brain tissue section samples. The laser pulse energy was kept constant for different repetition rates in order to encounter fluence dependent variations. For higher laser pulse repetition rates, mass spectral quality decreased and matrix-to-analyte signal intensity ratios increased for dried droplet and spray-coated mouse brain tissue section samples. CHCA showed a more pronounced repetition rate dependence compared to DHB, probably due to spectral absorption characteristics of CHCA. Overall ion intensities per laser pulse dropped when increasing the repetition rate from 60 Hz to 2000 Hz. In order to enhance measurement speed we optimized the number of laser pulses and the repetition rate for a continuous raster mode MSI with up to 10 pixel/s. High quality MSI data were obtained with pixel sizes down to 5 µm on mouse brain tissue sections. Future investigations will include experiments with other matrices in order to study and characterize the influence of the repetition rate on the MALDI process.

Acknowledgement

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New Aspects (25)

Implementation of a DPSS laser system for continuous raster MSI with an AP-SMALDI10 MSI system with ≥5 µm lateral resolution and 10 pixel/s.

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Getting DESI Imaging up to speed for clinical applications

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Introduction

Mass spectrometry imaging is an established analytical tool for biomolecular research by accurately localize molecules directly from a tissue section. To prosper in clinical research and pathological applications, imaging workflows need to be optimized with simple and robust sample preparation, fast acquisition rates/ high throughput and improved informatics to assess the imaging and mass spectral information quality the "on the fly" and/or rapidly after acquisition. Here we investigate optimisation of DESI imaging workflows with variation of acquisition speed in TOF and IMS mode along with the real time display of the ion images to assess image quality.

Methods

MS imaging experiments were performed using Waters Xevo G2-XS and SYNAPT HDMS G2-Si mass spectrometers. Images were recorded at different stage movement speeds and scan rates (1 scan/s, 10 scans/s 30 scans/s) at which meaningful results can be obtained. Furthermore, the implementation of real-time viewer prototype software enables the researcher to be informed of parts of the results while the system is still measuring. The 2D DESI experiments were carried out with and without ion mobility separation (IMS) in positive and negative mode. DESI analyses were run at 1.5 µl/min, 98:2 MeOH:water with gas pressure of 7 bar. DESI Imaging datasets were processed and visualized with the same software package called High Definition Imaging (HDI) 1.4.

Preliminary Data

Proof-of-principal experiments have been carried out using a thin section of sagittal mouse brain. Three rectangular regions were defined longitudinally along the brain tissue section. The surface of the tissue section was rastered line-by-line with mass spectra collected at predefined X,Y coordinates, initially in positive ion mode. The pixel size in the X direction was defined by the speed of the stage movement and acquisition rate of mass spectra. The Y-direction was defined by the distance between two lines of acquisition. All regions were imaged at a pixel size of 100 µm. The benchmark DESI imaging experiment acquired at 1 scan/s took 54 min. The increase of the acquisition speed to 10 scans/s decreased the acquisition time to 9 min and the fastest acquisition rate experiment took 6 min. However, as expected the signal intensities of the endogenous molecules decreased with the increase of the acquisition rate. Nevertheless the spectral resolution and mass accuracy was not affected with the variation of the speed of acquisition due to the decoupled nature of the ion source. A second experiment was carried out on the whole sagittal mouse brain in negative mode at 5 scan/s given high data quality in about 5 hours at 40 µm.

Further experiments will investigate the optimised acquisition rate in the case of DESI imaging acquisition followed by ion mobility separation (IMS) to increase the specificity of the experiment. To make the experiment faster, different raster modes can be implemented to decrease the time of stage movement.

Novel Aspect

Evaluation of a various speed continuous raster mode of DESI imaging on Q-TOF

Investigating the zinc distribution in the mayfly N. triangulifer using elemental bioimaging by LA-ICP-MS

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Introduction

Insects are an integral part of most freshwater and terrestrial food webs. Due to accumulation of environmental metals within their organism, they are also vectors transporting resources and contaminants across ecosystem boundaries. Thus, they endanger development and survival of consumers.

Metamorphosis from larvae to adult can cause chemical changes in insects. In general, metals are predominantly lost during metamorphosis leading to significantly higher concentrations in larvae compared to adult animals. Hence, there is a higher exposure risk for predators of larvae. In contrast, organic contaminants tend to accumulate in adults, causing higher exposure risks to predators of adult insects. This leads to the question how metamorphosis affects the distribution of contaminants between ecosystems.

Method

Experiments were performed with a 213 nm Nd:YAG laser using a spot diameter of 25 µm, which was coupled to the ICP-MS system by means of a transfer line. Possible interferences like [^{40}Ar+^{24}Mg] with ^{64}Zn were minimized utilizing a collision/reaction cell in kinetic energy discrimination (KED) mode with Helium as collision gas. The visualization was achieved by a line by line scan and subsequent merging. Laser parameters, including pulse energy, scan rate, and repetition frequency, were tuned for optimal signal intensity and spatial resolution.

Results and Discussion

In this study, the uptake and partitioning of zinc across five life stages of the mayfly Neocloeon triangulifer was investigated. The life stages include egg, late instar larvae (+ day 14), pre-emergent nymph (PEN- onset of metamorphosis), subimago (immature adult) and imago (sexually mature adult). Latter was measured pre and post egg deposition. To analyze the zinc distribution of naturally occurring zinc in different life stages, the flies were infiltrated in a sucrose solution, except the eggs. They were embedded directly in gelatin. For the frozen larvae a 30% sucrose solution was used. The flies of older life stages were

infiltrated in a 50% sucrose solution. After embedding the samples in gelatin, 14 µm thin cryosections were prepared. The metabolic zinc in the body of the mayflies was investigated by visualizing the different zinc distributions. Thus, images with a lateral resolution of 25 µm were generated. For quantification, an external calibration with gelatin standards in a range of 1 ppm to 500 ppm was used. The elemental mapping indicated, that the zinc concentration decreases during the different phases. Zinc is passing through the body and is likely shunted to the eggs in the ovaries.

Novel aspect

The uptake and distribution of metabolic zinc in different life stages of the mayfly N. triangulifer was examined by LA-ICP-MS.

Keywords
Imaging, LA-ICP-MS, metamorphosis, ecosystem

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Vortrag
Themen: Bildgebende Massenspektrometrie / MS Imaging
Stichworte: MS imaging, imzML, data processing, data standard, multimodal imaging

imzML - Current status and future perspectives of the open standard for mass spectrometry imaging data

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imzML is an open, vendor-neutral format for mass spectrometry imaging data [1]. It provides more flexibility in data processing as the user is no longer limited to proprietary software. Measurement results be shared between collaborators without loss of information. imzML is thus an important step towards more efficient collaboration and more transparent reporting in MS imaging. imzML has been launched in 2009. All relevant information including technical specifications, available software tools and implementation examples are provided on the website **www.imzml.org**. In recent years the imzML community has been very active and imzML has become the de facto international standard for mass spectrometry imaging data. Here we give an update on current activities and future perspectives of imzML.

Experimenteller Teil

imzML data consists of two files: a small file (XML) and a larger (binary) file. The XML file (.imzML) contains all relevant properties concerning the MS imaging experiments (position, pixel size...). The imaging binary data file (.ibd) contains the mass spectral data of the MS imaging measurement. We have converted a range of datasets from different mass spectrometer types (including Orbitrap, FTICR, Q-TOF, QqQ, TOF) and different vendors (Bruker, Thermo, Waters, Shimadzu, SCIEX, IonTOF). Conversion to imzML was performed by export functionalities in vendor software (FlexImaging by Bruker, ImageQuest by Thermo, HD Imaging by Waters) and software by academic groups (RAWConverter by U Giessen, toimzml module by CEA-LIST, imzMLConverter by U Birmingham).

Ergebnisse und Diskussion

The range of MS imaging software that supports imzML is constantly growing (see www.imzML for a complete list). The most recent additions in 2016 were ‘METASPACE’ by METASPACE consortium, ‘Spectral Analysis’ by University of Birmingham and ‘IonView’ by Shimadzu. In our lab we have tested 14 different software tools that support imzML for data analysis and visualization. This includes open source, freely available and commercial packages. We were able to open and process imzML files in all of these software tools. Each of them offers unique features. We will give a brief overview of functionalities and also explain limitations/restrictions, e.g. some software tools are only able to process ‘CONTINOUS’ data.

We have developed a new conversion tool that allows integration of vibrational spectroscopy data (or any other csv formatted data) in the imzML workflow. We will demonstrate this on an example of MALDI, Raman and FTIR imaging of a single tissue section.

imzML data can also be submitted to PRIDE database (www.ebi.ac.uk/pride/archive/) enabling a public data repository and ‘open data’ examples for mass spectrometry imaging [2]. A similar functionality is currently being implemented in other repositories.

Another application of imzML is the comparison of data from multi-center studies, which allows to display data from different instruments in one software with identical settings for visualization (e.g. color scale and interpolation) [3]. We will present a combination of SIMS and MALDI which includes an imzML dataset that was generated from 4.2 million spectra of a TOF-SIMS instrument. The maximum number of spectra is mainly limited by hardware resources and not by software (anymore). Future developments will also be discussed, for example the integration of 3D and ion mobility data in imzML.

Neue Aspekte

imzML-based data processing strategies, including public repository, multicenter studies. New generic conversion tool. First conversion of 4+ million spectra dataset.

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Energetische und kinetische Betrachtung der Fragmentierung von Azofarbstoffen mit Diethylamino Gruppe

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Einleitung

Fragmentierungsprozesse von Molekülen sind von grundlegendem Interesse für die Physikalische Chemie und vielen angrenzenden Disziplinen. Die Energieaufnahme und deren Umverteilung auf Schwingungsfreiheitsgrade beeinflussen die Fragmentierung maßgeblich. Zur Aufklärung von Fragmentierungsmechanismen sind Kenntnisse über diese Prozesse nötig.
Neben Rhodamin B [1,2] zeigen weitere Moleküle [3], u.a. Azofarbstoffe, unerwartete Fragmentierungsreaktionen. Der Verlust von C_3H_8 aus einer Diethylamino Gruppe kann nicht aus der Struktur selbst erklärt werden. Verschiedene Reaktionswege sind möglich. Das kann zum einen eine konzertierte Reaktion über einen cyclischen Übergangszustand sein. Zum anderen ist eine konsekutive radikalische Reaktion denkbar. Allein massenspektrometrisch sind beide Reaktionswege nicht eindeutig zu unterscheiden. Für die Interpretation der Fragmentierungsmechanismen der Azofarbstoffe wird eine Kombination aus Massenspektrometrie, quantenchemischen und RRKM Rechnungen verwendet.

Experimenteller Teil

Die Aufnahme aller Massenspektren erfolgte mit einem *APEX-IV Qe* FT-ICR Massenspektrometer mit einem 9.4 T supraleitenden Magneten (*Bruker Daltonik*, Bremen, Deutschland). Alle Analyten wurden in Ethanol gelöst, mit einem Lösungsmittelgemisch aus Methanol/Wasser/Ameisensäure verdünnt und anschließend mittels Elektrospray Ionisation in die Gasphase gebracht.
Zwei Methoden wurden zur Fragmentierung der isolierten Ionen verwendet. Zum einen konnte ein Argon-Ionen-Laser (*Innova 70*, Coherent, Santa Clara, CA, USA) im *multiline* Modus für die Photodissoziation im sichtbaren Wellenlängenbereich (VisPD) verwendet werden. Des Weiteren konnten die gespeicherten Ionen mittels Stoßgas (Argon) angeregt und fragmentiert werden.
DFT Rechnungen der Reaktionswege wurden mit dem *Gaussian 09* Paket durchgeführt. Hierfür wurde das Funktional B3LYP mit dem Basissatz 6-311+G(2df,2pd) verwendet.

Ergebnisse und Diskussion

Ethylrot (4-(Diethylamino)azobenzol-2'-carbonsäure) zeigt keine direkte Abspaltung von C_3H_8 aus dem Molekülion ($[M+H]^+$). Es kann ein kombinierter Verlust aus H_2O und C_3H_8 beobachtet werden. Das Fragmentierungsmuster zeigt, dass mehrere Reaktionspfade zur Abspaltung von C_3H_8 führen. Auf den Verlust eines Methylradikals folgt der Verlust eines Ethylradikals und führt in Kombination mit dem Wasserverlust zum Fragmention $[M+H-C_3H_{10}O]^+$. Weiterhin ist eine Cyclisierungsreaktion des Ethylrots im Zuge der Wasserabspaltung denkbar. Deutliche Hinweise darauf liefert der Verlust von N_2, der in Kombination mit weiteren Abspaltungen auftritt. Es kann ein Fragmention beobachtet werden, das durch Verluste von Wasser, Stickstoff und einem Methylradikal gebildet wird. Ein wiederum folgender Verlust eines Ethylradikals führt zur Spezies $[M+H-C_3H_{10}N_2O]^+$. Diese beiden Fragmentierungsreaktionen zeigen, dass der Verlust von C_3H_8 aus der Diethylamino Gruppe konsekutiv abläuft. Nichtsdestotrotz schließen diese Beobachtungen das Ablaufen einer konzertierten Reaktion, die zu denselben Fragmentionen führt nicht aus. Des Weiteren ist unklar, warum als radikalische Zwischenprodukte nur Fragmente nach einem Methylradikalverlust auftreten und keine nach einem Ethylradikalverlust.
Die energetische Betrachtung der möglichen Fragmentierungsreaktionen liefert hierbei weitere Hinweise. Für das Ethylrot kann gezeigt werden, dass der Verlust eines Methylradikals gegenüber dem Verlust eines Ethylradikals bevorzugt stattfindet. Dies kann durch die bessere Resonanzstabilisierung des entstehenden Fragmentions bei dem Verlust eines Methylradikals erklärt werden. Die konzertierte Fragmentierungsreaktion über einen cyclischen Übergangszustand ist energetisch ebenfalls denkbar und hilft nicht bei der Unterscheidung dieser zwei Reaktionswege. Neben der Energetik ist auch die Kinetik entscheidend, ob Fragmentierungsreaktionen ablaufen können oder nicht. Kinetische Berechnungen, die auf der RRKM Theorie beruhen, zeigen hierbei für die denkbaren Fragmentierungswege Unterschiede auf. Der radikalische Fragmentierungsmechanismus findet demnach deutlich bevorzugt statt. Demgegenüber ist der konzertierte Fragmentierungsmechanismus kinetisch gehindert, so dass dieser sehr wahrscheinlich nicht abläuft.
Ebenso kann das Fragmentierungsverhalten von Ethylgelb (4-(Diethylamino)azobenzol) untersucht werden. Im Gegensatz zum Ethylrot kann in diesem Fall die Bevorzugung eines Ethylradikalverlustes aus der Diethylamino Gruppe beobachtet werden.

Neue Aspekte

Es ist erstmalig möglich konsekutive und konzertierte Fragmentierungsreaktionen der Diethylamino Gruppe mittels Massenspektrometrie, energetischer und kinetischer Betrachtungen zu unterscheiden.

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Stichworte

Hochauflösende Massenspektrometrie; Fragmentierungsreaktionen; Photodissoziation; DFT; RRKM

COPPER-CATALYSED CLICK REACTION PERFORMED IN THE GAS PHASE: A COMBINED MASS SPECTROMETRIC AND DFT MECHANISTIC STUDY

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Introduction

The copper-catalysed azide–alkyne cycloaddition (CuAAC)[1] is the most prominent example of the so-called "click chemistry". The robustness of this CuI-mediated transformation has boosted its interest, making it the most straightforward strategy for the regiospecific preparation of 1,2,3-triazoles. To date, this reaction is widely employed in organic synthesis, medicinal chemistry, surface and polymer science, and in bioconjugation strategies. Despite the apparent simplicity and widespread use of the reaction, its mechanism has emerged as particularly complex, being still a matter of debate. Despite many mechanistic studies, only recently the key role of bis(copper) complexes in the catalytic cycle was experimentally demonstrated.[2]

In this field, ion/molecule experiments (collision activated reaction (CAR)) on organometallics by MS are powerful tools to investigate reaction mechanisms.[3]

Experimental

We modified a triple quadrupole mass spectrometer (Quattro II, Waters/Micromass) to perform sequential ion/molecule reactions on bis(copper) adducts, in order to reproduce the catalytic cycle of CuAAC in the gas-phase. In particular, we turned the first transfer hexapole (H0) into a closed collision cell which incorporates two gas inlets. They are connected with two glass flasks by means of micrometric valves. Volatile reactants can be placed into the flasks and a finely adjusted flow of their vapours can be sent at two different stages of H0 and/or H1. This configuration allows copper adducts, formed at the spray source stage, to collide with CuAAC reactants (phenylacetylene and/or benzylazide taken in via the two inlets) to perform consecutive CAR/CID, and CAR/CAR/CID experiments.[4]

Results and discussion

A DCM solution of CuOTf and PPh_3 was electrosprayed and the naked $[Cu_2OTf]^+$ ion was generated by in-source fragmentation. It was then collided with phenylacetylene in H0 to generate a monocoordinated adduct (computed stabilization energy=244.35kJ/mol. The resulting alkyne complex was then isolated in Q1 and left to collide with argon in H2. Under CID conditions it undergoes the first proton transfer of CuAAC pathway leading to the dissociation of a triflic acid unit and to the formation of the key bis(copper) acetylide intermediate.

Once having generated the bis(copper) acetylide in the gas-phase we turned our attention on its reactivity toward azides. To this end bis(copper) acetylide intermediate was ionized by ESI from a DCM solution containing Cu–≡–Ph, Cu(OTf), and PPh_3. It was submitted to CAR/CAR experiment in H0 filled in with benzylazide (1st gas inlet) and trifluoroacetic acid (2nd gas inlet). Trifluoroacetic acid has been chosen as volatile proton source needed for the final protonolysis stage of CuAAC. Keeping Q1 static, the resulting adduct, formed in H0, was mass-selected and allowed to decompose in H2 under CID conditions. Under such conditions the cycloaddition occurred leading to the formation of the final triazole product.

Interestingly, the presence of one phosphine ligand on the initial bis(copper) acetylide intermediate was strictly required for the cycloaddition in the gas-phase. It probably enhances the proximity of the triple bond and the azide coordinated under CAR conditions as also suggested by DFT calculations.

The role of the ancillary ligand was further investigated by interrogating the gas-phase reactivity of the bis(copper) acetylide containing two PPh_3 molecules or a bidentate phosphine.

Finally, we also synthesised an imidazolium-tagged alkyne to interrogate the reactivity of mononuclear copper acetylide, with or without phosphine ligands. Mononuclear acetylides were unreactive toward benzylazide under our gas-phase conditions.

Novel aspects

A triazole product has been synthesised in the gas-phase by sequential ion/molecule reactions through a series of bis(copper) intermediates.[4]

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Electrospray Fourier Transform ion cyclotron resolution mass spectrometry (FT-ICR MS): reactivity of polyaromantic heterocycles in heavy crude oils towards benzyl halides.

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Introduction

The petroleum refining trends are shifting toward production of heavier crude oils. Compared to the lighter crudes, they contain higher amounts of unwanted hetero- (N-, S-, and O-) aromatic components which are deleterious and harmful for refining catalysts and environments. A detailed knowledge of the distribution of the hetero-atomic compounds in crude oils and the structural information is necessary to improve their removal processes. Benzyl halides, as the first time, are introduced for the selective analysis towards specific heteroatom class in a whole crude oil with FT-ICR MS under positive electrospray conditions; vice versa, crude oil, as a *supercomplex* mixture substrate system, has a wealth of functional and structural information, challenging the organic chemists besides the analysts.

Method

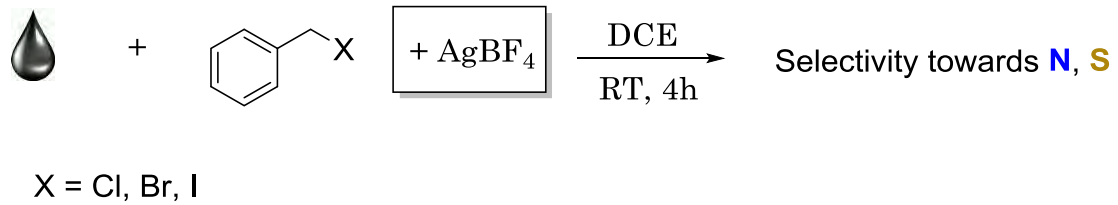
A heavy crude oil was dissolved in dry 1, 2-dichloroethane (DCE) and was reacted with a certain amount of benzyl halides (C_7H_7X) in the presence of silver tetrafluoroborate ($AgBF_4$) for 4 h. The precipitate was removed by centrifugation and washed with DCE.

Dibenzothiophene (DBT) was dissolved in dry DCE and was reacted with a certain amount of C_7H_7X for 4 h; the same procedure was carried out for a heavy crude oil.

Mass spectra were recorded using a 7 T FT-ICR MS (Thermo Fisher Scientific, Bremen) and a high-field Orbitrap FTMS equipped with an ESI source. ^{1}H NMR spectra were recorded on a Bruker Advance 300 NMR spectrometer.

Results and discussion

ESI is a widely used ionization method that covers a broad range of components, often with a higher polarity. Benzyl halides are introduced to study the selective derivatization of crude oil as shown in Scheme 1, which allows ionizing non-polar components such as sulfur-containing compounds that are not ionizable by electrospray.



Scheme 1: Benzylation of a heavy crude oil

Under positive ESI, polar basic N_1 and N_1S_1 species are the most widely appearing classes in the original heavy crude oil. The flip happened after the benzylation of heavy crude oil with the presence of $AgBF_4$, the sulfur-containing compounds such as S_1 and S_2 classes are being detected over nitrogen-containing-species to be accessed with a high degree of selectivity, especially in reactions of benzyl chloride and benzyl bromide. In the case of benzyl iodide, although S_1 is the dominant class, the relative abundance of NS_2 increases by a factor of 7. The NS_3-classcan be detected in a reactionof benzyl iodide and benzyl bromide.

Benzylation of heavy crude oil without the presence of $AgBF_4$ under positive ESI has also been investigated. Benzyl iodide highly facilitates the selective detection of sulfur-containing compounds including the S_1, S_2 and S_3 classes, and the S1 class spans a DBE range of 3-25; while benzyl chloride aids only nitrogen-containing compounds including N_1, $N_1O_1S_1$, N_1S_1, $N_1O_1S_2$ classes detectable, and N_1O_1S class was detected as a new heteroatom class compared to the original crude oil; both sulfur-containing species (S1, S2, S3 classes) and nitrogen-containing species (N_1, N_1S_1, N_1S_2, $N_1O_1S_1$ classes) are observed in the case of benzyl bromide. ^{1}H NMR spectra obtained from the mixture of standard DBT with three benzyl halides are used to understand the mechanism of the reaction.

Novel aspects

Benzyl halides are introduced for selective derivatization of crude oil by FT-ICR coupled with ESI.

Keywords

Electrospray ionization, FT-ICR mass spectrometry, benzyl halides, selective analysis, crude oil.

Internal energy of ions produced by electrospray and cryospray ionization

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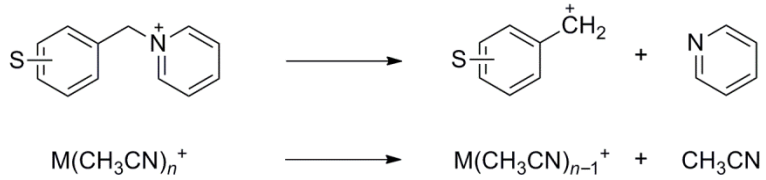
Cryospray ionization (CSI), a variant of electrospray ionization (ESI), uses a cooled nebulizer and drying gas to prevent the unwanted decomposition of thermolabile analytes during the ionization process [1]. Despite the great potential of this method, its performance has not been investigated sytematically yet. In particular, it is unclear to which extent CSI lowers the internal energies of the produced ions.

A simple and well-established method to determine the effective internal energies of ions relies on so-called thermometer ions, whose fragmentation indicates that their internal energies exceed their dissociation threshold [2]. By correlating the ratio of fragmented and intact ions with the dissociation energies of the latter, the effective internal energies of the ions could be determined according to the so-called survival-yield method [2]. For the characterization of the ESI process, most commonly benzylpyridinium ions are used as thermometer ions [2].



After a re-evaluation of their dissociation energies and the kinetic shifts associated with their fragmentation, we have applied these systems to the present problem. Due to their rather high dissociation energies, they are of only limited use for determining the relatively low internal energies of ions produced under mild conditions. Therefore, we have also considered micro-solvated alkali-metal cations $M(CH_3CN)_n^+$ as alternative thermometer ions with lower dissociation energies. With these systems, we have been able to determine the effective internal energies imparted by the ESI and the CSI process, respectively. Surprisingly, we have found almost identical internal energy distributions in both cases. This result suggests that under typical conditions, the internal energies of the ions are not controlled by the ionization process itself, but by the occurrence of energetic collisions between the ions and residual neutrals in the ion-transfer region of the mass spectrometer. For the investigation of thermolabile analytes, a rigorous cooling of the sample solution may therefore be more important than the use of CSI instead of simple ESI.

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Keywords: cryospray ionization, electrospray ionization, internal energy, thermometer ions

Mapping metabolites from rough terrain: laser ablation electrospray ionization on non-flat samples

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Introduction

To guarantee optimal laser focus during laser-based ionization experiments, the sample is required to be as flat as possible. When analyzing surfaces of insects, bacterial colonies or plants, the requirement of flatness is rarely met. So far, the effects of surface topography on consistent laser ablation in mass spectrometry imaging are largely ignored. Profilometry [1] offers the possibility guide laser ablation in the 3rd dimension by recording height profiles of surface topography prior to laser-based ionization experiments.

Methods

Topographic maps of sample surfaces were generated using an in-house developed R script from data acquired with a confocal distance sensor (µ-Epsilon). Metabolic profiling of the samples was performed subsequently with a custom-built laser ablation electrospray ionization source [2,3] connected to a LTQ Orbitrap mass spectrometer (Thermo Scientific). Laser focus was maintained by adjusting the sample's position in the 3rd dimension based on the recorded height profiles. Pseudo-colored ion intensity maps were generated from the acquired MS-spectra.

Results

A telescope infrared-laser optic was employed in a custom-built laser ablation electrospray ionization source to focus an OPO-pumped pulse laser operating at 2940 nm wavelength. Height profiles of Raphanus sativus (radish, piccolo cultivar) leaves were recorded with a lateral resolution from 200 µm down to 10 µm using the confocal sensor. The recorded height profiles were applied to perform metabolic profiling/imaging on radish leaf surfaces with topographic features differing in height up to 1400 µm. Consistent laser ablation was performed with a laser-ablation-mark diameter of 70 µm in average [3]. Without topographic guidance, ablation mark diameter doubled within 200 µm above and below the focal plane. All processes are integrated in LabVIEW software and the measurements are executed automatically. Using R scripts, the resulting data files were integrated into a data cube for visualization.

Novel Aspect

Height profiles of biological samples recorded prior to IR-Laser ablation to achieve constant laser focus without cross-sectioning for unbiased profiling/imaging.

Topics

LAESI, MSI, Profilometry

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ID: 27 / MoV_3b: 3
Vortrag
Themen: Grundlagen der Massenspektrometrie, Ionisationsmethoden
Stichworte: MALDI, desorption, ablation, spot size dependence, velocity distribution

New insights into the MALDI mechanisms: Postionization and photoacoustic experiments reveal laser spot size-dependent transitions between desorption and ablation regimes

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For MALDI mass spectrometry, laser spot sizes ranging between about 100-200 µm by diameter in typical proteomics applications down to a few micrometers in high-resolving MALDI-MS imaging experiments are utilized. Numerous studies indicated a peculiar "spot size effect", i.e., an over-proportional increase of the ion detection fluence thresholds with decreasing spot size [e. g. 1, 2]. However, the underlying mechanisms remained largely unclear. Here we recorded the spot size- and fluence-dependence of the neutral material ejection using complementary photoacoustic [3] and MALDI-2-like postionization [4] setups. Moreover, a fundamental beam shaper [2] was used to compare flat-top and Gaussian intensity spots. The results reveal a transition from primary molecular desorption at larger to primary bulk material ablation at smaller spot sizes.

Experimenteller Teil

Microcrystalline layers of 2,5-dihydroxybenzoic acid (DHB) or α-cyano-4-hydroxycinnamic acid (HCCA) matrices were sublimated/recrystallized onto sections of homogenized pig brain tissue. Q-switched Nd:YAG (λ=355 nm) and Nd:VYO_4 lasers (349 nm) of high beam quality served as light sources. Focal diameters were adjusted between approximately 5-200 µm using telescope optics and a beam profiler. MS data were recorded with a Synapt G2-S QTOF mass spectrometer, equipped with a postionization (PI) laser [4] for probing ejected analyte (lipid) and matrix molecules at 280 nm wavelength and a central sample-to-PI laser beam distance of ca. 500 µm. Photoacoustic data, reflecting the material ejection-derived pressure waves, were recorded at atmospheric pressure using a custom-made cell and using an evaluation strategy as described previously [3].

Ergebnisse und Diskussion

For both matrices and Gaussian as well as flat-top beam profiles, a transition between desorption and ablation regimes of the overall material ejection process was revealed by the photoacoustic measurements and for DHB also with the postionization setup (HCCA not measured). The plume dynamics were found to depend on both the focal laser spot size, with a transition zone found between 40 and 90 µm spot diameter, and the laser fluence. In particular, our extensive PI experiments, in which not only a vast fluence range was covered, but also the delay between the two laser pulses varied between 100 ns and 100 µs, enabled detailed insight into the plume expansion dynamics and revealed a bimodular characteristic. For the large spot size regime (above ~80-90 µm in diameter) and typical MALDI fluences, the analyte/matrix plume was rapidly expanding with mean velocities of both lipid analyte and matrix molecules close to 1000 m/s, in good agreement with previous results and quasi-

thermal model considerations [3, 5]. For spot sizes in the transition range from 40–90 µm and/or elevated fluences two maxima were found, where the second presumably reflects clusters with mean velocities of only a few ten m/s. Assuming similar kinetic energies as the monomeric plume constituents, analyte/matrix compositions of ~500-2000 molecules/cluster would be derived – a size that fits reasonably well with molecular dynamic simulations of MALDI-like scenarios [5]. For the smallest tested spot sizes in the 10 µm-range, only the slow plume component was found. In line with the previous results [1, 2], in this regime elevated fluences are required to produce enough material, even for MALDI-2 postionization. Next to providing new insights into the spot size effect in MALDI our results could be helpful for further refinement of MALDI and MALDI-2 ion sources and the development of efficient high-resolving MALDI-MSI.

Neue Aspekte

Detailed experiments on the spot size effect in MALDI providing an answer to a long-lasting question about the MALDI mechanisms

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Selective triacylglycerol suppression in complex lipid mixtures by CsCl addition

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Einleitung

Ion suppression is a known disadvantage in mixture analysis. Spectra of complex lipid mixtures are often dominated by signals of phosphatidylcholines (PC). However, adipose tissues contain huge amounts of triacylglycerols (TAG) but only minor amounts of phospholipids such as PC or particularly phosphatidylethanolamines (PE). Therefore, mass spectra of crude adipose tissue extracts are dominated by TAG signals while less abundant PLs (PCs and particularly PEs) are suppressed.

MALDI MS has a high tolerance towards salts and this enables the application of "auxiliary agents" such as selected salts. This study shows that the saturation of the MALDI matrix solution with solid CsCl is a simple to perform approach to overcome the ion suppression effect of TAGs in adipose tissue extracts [1].

Experimenteller Teil

The solvents, triolein and the MALDI matrix (2,5-dihydroxybenzoic acid; DHB) as well as NaCl, KCl, RbCl and CsCl were obtained from Sigma-Aldrich (Taufkirchen, Germany) in the highest commercially available quality and used without purification [2]. All phospholipid standards were obtained from Avanti Polar Lipids as 10 mg/mL solutions in $CHCl_3$ and diluted to the required concentration. DOTAP (1,2-dioleoyl-3-trimethylammonium-propane (chloride salt)) was used in selected cases as internal MS standard.

All animal experiments were performed according to the German national guidelines of laboratory animal care. Tissue lipids were extracted by using methyl-tert-butyl ether (MTBE) [3]. All lipid samples were analyzed by means of MALDI MS (Bruker Autoflex) and ^{13}C HR NMR (Bruker DRX 300 at 75.45 MHz).

Ergebnisse und Diskussion

Adipose tissues are extremely rich in triacylglycerols. The TAG content accounts for about 95% of the total lipids, while phospholipids (predominantly PC) make out only about 5%. Therefore, the excess of TAG leads to the suppression of less abundant tissue (phospho)lipids [4].

An artificial mixture of triolein, POPC and POPE was initially investigated, in order to mimic adipose tissue composition, followed by brown adipose tissue extract. The influence of different alkali metal chlorides on detection of PL and TAG signals was analyzed in each case.

Saturation of the DHB matrix with solid CsCl leads to tremendous differences in mass spectra: a significant reduction of the TAG signal intensities and, concomitantly, a considerable increase of the intensity of small signals of phospholipids. The decrease of the TAG intensity is particularly caused by (a) the increased fragmentation of the corresponding alkali metal adducts and (b) the considerable size of the Cs^+ ion which prevents successful analyte ionization. The effect of CsCl addition on the TAG peak intensities was observed in artificial lipid mixtures of known compositions as well as in biologically relevant lipid mixtures. Using an excessive salt concentration is important to minimize the influence of the matrix. Nearly identical data can be obtained with equimolar ratios between salt and matrix.

We suggest that the observed differences are caused by the different sizes of the alkali metal ions. In order to elucidate this effect the measurements were repeated in the presence of different alkali chlorides with increasing sizes.

This study shows that addition of CsCl is a useful method to overcome ion suppression of phospholipids in samples with an excess of TAGs. This analysis can be performed rapidly and without the need for previous separation of the samples, is highly time-saving and provides reliable compositional information in a single measurement.

Neue Aspekte

The addition of CsCl improves the detectability of small amounts of phospholipids in the presence of an excess of TAG.

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DGMS 2017

Elemental Bioimaging by LA-ICP-QQQ-MS for the Investigation of Wilson´s Disease

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Einleitung (120 Wörter)

Wilson´s disease (WD) is a rare genetic disorder of the copper metabolism, causing the accumulation of copper in different organs, including liver, central nervous system and cornea. This way, WD initiates manifold hepatic, neurological or psychiatric symptoms. In the contemporary medicine, chelation therapy is applied to remove excess copper from the organism of WD patients. To learn about the elemental distribution in liver samples after chelation therapy, liver samples from human WD patients and from LEC rats, an animal model for WD, were analyzed by laser ablation-inductively coupled plasma-triple quadrupole-mass spectrometry (LA-ICP-QQQ-MS). In comparison to single quadrupole ICP-MS, ICP-QQQ-MS allows interference removal in reaction mode and therefore an improved detection of otherwise difficult elements such as sulphur.

Experimenteller Teil (120 Wörter)

Within this work, human WD liver samples from patients following D-penicillamine (DPA) chelation therapy as well as liver samples from LEC rats treated with novel chelation compounds were investigated. To study the elemental distribution in liver samples, LA-ICP-QQQ-MS was applied as imaging technique. The ablation was performed with a 213 nm Nd:YAG laser using a spatial resolution of 10 µm and a scan rate of 20 $\mu m \cdot s^{-1}$. Using the ICP-

QQQ-MS in reaction mode in order to avoid interferences, sulphur, iron, copper, and zinc were monitored within the liver samples. All elements were quantified using homemade matrix-matched standards made of gelatin.

Ergebnisse und Diskussion (300 Wörter)

The presented LA-ICP-QQQ-MS method provides a valuable tool for the investigation of the elemental distribution in liver tissue. Using ICP-QQQ-MS in reaction mode with 30% O_2 in H_2 as cell gas, low detection limits for additional elements such as sulphur, which is known to be difficult in conventional single quadrupole ICP-MS, can be achieved. In this work, inhomogeneous sulphur distribution maps within the analyzed liver samples were detected. Serving as an example, an DPA treated human WD liver sample showed a correlation of areas with an increased sulphur, iron and zinc concentration, while a wash-out of copper in proximity to blood vessels is indicated. Generally, LA-ICP-MS is an excellent methodology for the evaluation of the efficacy of current and novel chelation therapies of WD, while triple quadrupole ICP-MS proves to be a powerful system to remove interferences in reaction mode. The results of this work may contribute to a better understanding of WD itself and the chelation effect in the treatment of WD.

Neue Aspekte (20 Wörter)

Bioimaging of the sulphur distribution in Wilson´s disease liver samples by LA-ICP-QQQ-MS.

Stichworte (Maximal 5 durch Kommata getrennte Stichwörter)

Triple quadrupole ICP-MS, Laser ablation, Wilson´s disease, Sulphur

Kategorie (Bis zu zwei)

Element-Massenspektrometrie, MS-Imaging

Electrochemical conversion of Pt(IV) prodrugs to Pt(II) cytostatics investigated by means of liquid chromatography and mass spectrometry

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Introduction (max. 120)

Platinum containing cytostatics represent an important class of chemotherapeutics during cancer treatment. Clinically, Pt(II)-based species such as Cisplatin, Carboplatin or Oxaliplatin are applied. However, those cytostatics show low selectivity towards tumor tissue why current research focuses on alternative compounds entailing less side effects. One approach is based on Pt(IV) complexes which are more stable and could serve as a prodrug for Pt(II) cytostatics. The addition of certain structural properties to the axial ligands of Pt(IV) compounds could enhance the tumor uptake leading to an enrichment in the tumor cells. For this reason, the Pt(IV) compound should be predominantly reduced in the tumor and thus, targeted chemotherapeutic treatment could be achieved.

Method (max. 120)

In order to simulate the *in vivo* occurring reduction processes of Pt(IV) prodrugs a purely instrumental setup consisting of an electrochemical thin-layer cell coupled to liquid chromatography (LC) and mass spectrometry (MS) was applied. By this means, the electrochemical reduction of three novel Pt(IV) compounds as well as Satraplatin was performed and the products were characterized using LC-electrospray (ESI)-MS and LC-inductively coupled plasma (ICP)-MS. Further investigations on the influence of the different axial ligands and the central molecules of the Pt(IV) compounds to the reduction efficiency were carried out by application of post-column isotope dilution analysis.

Results and discussion (max. 300)

The release of Pt(II) cytostatics from Pt(IV) prodrugs was investigated by means of electrochemistry (EC) coupled to LC-MS in order to simulate the *in vivo* occurring reduction processes. All species were electrochemically reduced in high yields using a commercially available analytical thin-layer cell followed by an (LC-)ESI-MS analysis in order to obtain molecular information. Complementary, LC-ICP-MS analysis was carried out resulting in elemental information for platinum. Evaluation of the reduction behavior of the compounds based on their different axial ligands and the central molecules was performed by post-column isotope dilution. In all cases, the desired reduction product represent the most prominent species detected with an amount of 66-73% of total platinum obtained after electrochemical reduction. However, no significant differences in the reduction efficiencies of the Pt(IV) compounds could be determined based upon their different ligands or central molecules. Nevertheless, coupling of reductive electrochemistry to LC-MS has been figured out to be a powerful tool for a fast and easy reduction of small molecules such as Pt(IV) prodrugs without the need of time-consuming and expensive animal models.

New aspects (max. 20.)

The electrochemical reduction of novel Pt(IV) prodrugs to Pt(II) cytostatics was investigated using LC-MS and resulted in high yields.

ID: 44 / MoV_4a: 3
Vortrag
Themen: Proteine & Proteomics, Lebensmittelanalytik
Stichworte: Oxidation, Protein carbonylation, Aldehyde reactive probe, Milk proteomics

Protein carbonylation in raw milk and differently processed milk products

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Pasteurization and ultra high temperature treatment of milk guarantee its microbiological safety and extended shelf-life times, but also can induce oxidations of milk proteins, e.g., carbonylation. Protein carbonylation is a non-enzymatic modification widely accepted as a biomarker of oxidative stress, but is poorly studied in milk although it can affect the milk proteins at different residues and by different reactions. Protein-bound carbonyls can be formed by metal-catalyzed oxidation (MCO) of certain residues in the presence of reactiveoxygen species; as adducts with dicarbonyls or reactive carbonyls formed as lipid peroxidation products (LPPs). These modifications compromise the quality and nutritive value of milk, but may also initiate pathological processes, allergic reactions or activate receptors.

Experimenteller Teil

Oxidative damage of milk proteins induced by industrial processing was evaluated by the identification of carbonylation sites in raw and differently processed milk products including different brands of pasteurized (three brands), ultra high temperature (UHT, three brands) treated milk and infant formulas (IFs, five brands). Milk proteins were precipitated from two replicates of each milk sample and digested with trypsin. Carbonylated peptides were derivatized with aldehyde reactive probe (ARP), enriched by biotin-avidin affinity chromatography, and analyzed by targeted nRPC-ESI-MS/MS using DDA top 6 (CID mode) after excluding previously identified unmodified peptides. Modified peptides were identified with high confidence scores by Sequest and confirmed by manually checking the tandem mass spectra.

Ergebnisse und Diskussion

In total, 53 unique carbonylated peptides representing 37 carbonylation sites of 15 proteins were confidently identified in milk samples. The CID tandem mass spectra allowed the identification of different types of carbonyl modifications with high confidence, i.e., glyoxal, methylglyoxal or 3-deoxyglucosone adducts on Lys, Cys and Arg (dicarbonyl-derived modifications), acrolein, pentenal, 4-oxo-2-hexenal (OHE) on Lys (α,β-unsaturated aldehydes - LPPs), aminoadipic semialdehyde on Lys, and glutamic semialdehyde on Pro (metal-catalyzed oxidation). κ-Casein and whey proteins β-lactoglobulin and α-lactalbumin were identified with the highest number of carbonylation sites. Most modifications (57%) were located on lysine residues, whereas the rest were distributed on Cys (17%), Pro (14%) and Arg (12%).

Glyoxal-derived carbonyls were the major modification type on Lys, Cys, and Arg accounting for 90% of the total number of dicarbonyl-derived modification sites. Thus, it was the main carbonylation route in processed milk products (70%, 26 unique modification sites in 12 milk proteins), followed by MCO (24.3%, nine modification sites in three proteins) and adducts with α,β-unsaturated aldehydes (LPPs) (16.2%, six sites in four proteins). The total number of dicarbonyl-derived carbonylation sites was significantly higher in thermally processed samples and increased from raw colostrum (one) and raw milk (four) to pasteurized and UHT milk (16) to IF (24). Relative quantification of several glyoxal-modified peptides supported this trend. κ-Casein and α_{S1}-casein were the main targets of MCO. Interestingly, five out of the six glutamic semialdehydes were identified on proline residues of κ-CN. In addition, α,β-unsaturated aldehydes (acrolein, OHE, and pentenal) modified six residues in four proteins. Interestingly, several residues were carbonylated by different pathways.

Neue Aspekte

Thirty-seven novel carbonylation sites were identified in fifteen bovine milk proteins.

Entwicklung einer LC-MS/MS Methode zur Bestimmung der Backdoorpathway Hormone Androsterone und Androstandiol und der Androgene Androstendion, Testosteron und Dihydrotestosteron

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Einleitung:
Bei dem Tammar Wallaby konnte von Wilson et al. [1] ein weiterer Synthesweg zum Dihydrotestosteron (DHT) unter Umgehung des klassichen Hormone Testosteron und Androstendion gezeigt werden. Die menschliche Enzymausstattung kann diese alternativen Konvertierungen ebenfalls ermöglichen[2]. Kamrath et al.[3] konnten die Backdoorpatwhway-Steroide im Urin von Patienten mit 21-hydroxylase Mangel (21OHD) nachweisen. Mit 95% ist der 21-Hydroxylase-Mangel (21OHD) die häufigste Form des Adrenogenitalen Syndroms und führt u.a. partielle Nebenniereninsuffizienz.
Ziel war die Entwicklung einer neuen LC-MS/MS-Methode zur parallelen Erfassung von Androsterone, Androstandiol, Androstendion, Testosteron und DHT und der Nachweis der Steroide bei Kindern.
Methoden:
0,1 mL Plasma wurden mittels Festphasenextraktion und LC-MS/MS-Massenspektrometrie analysiert. Die Hormone wurden in einem Referenzkolletiv bestehend aus 97 Kindern (38 Mädchen, 59 Jungen), 0-20 Jahren. Das 21-OHD-Kollektiv umfasst 117 21OHDPatienten (47 Mädchen, 70 Jungen), 0-20 Jahre.
Ergebnisse und Diskussion:
Für jedes Hormon werden zwei MRM-Spuren gemessen. Die Bestimmungsgrenzen der Hormone liegen zwischen (0.02 nmol/L) (Testosteron) und (0.12 nmmol/L) (Androstandiol). Die Hormone des BP finden sich sowohl in Messungen des Normalkollektives als auch bei 21-OHD-Patienten. 21OHD-Patienten haben signifikant höhere Plasmakonzentrationen von DHT (Mädchen, MW 0,56 nmol/l 21OHD, 0,13 nmol/l Referenz, p <0.001, Jungen: 0,75 21OHD, 0.58 nmol/l Refernz, p <0.001, 56,2 ng/dL Referenzkolletiv, p 0.03). Bei Jungen sind zusätzölich noch signifikant höhere Werte für Androstandiol messbar (MW 3.7 nmol/L 21OHD, 1.9 nmol/L referenz, p 0.0003).
Backdoorpathway Hormone sind im kindlichen Plasma messbar und beim AGS mit 21-OHD signifikant höher konzentriert. Eine mögliche Rolle der BP-Steroide zum Monitoring einer AGS-Einstellung bedarf nach dieser Phase der Methodenimplementierung klinischer Studien.

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Vitamin D_3 epimers: analytical nuisance or clinical opportunity?

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Introduction

Vitamin D status is determined by circulating 25-hydroxyvitamin D levels, since this metabolite is directly linked to vitamin D substrate availability. An alternative parallel metabolism pathway encompassing C-3 epimerization was discovered, which questioned whether the epimerized vitamin D metabolites have their own biological functions, which is currently unknown. The epimers result from reversal of the stereochemical configuration of the C-3 hydroxyl group. Contrary to the primary C-3β metabolite, the C-3α epimer exhibits little or no calcemic effects; its presence therefore overestimates serum vitamin D status, unless adequately accounted for. This presentation highlights analytical and mass spectrometric difficulties when measuring the two epimers, but also presents solutions to accurately quantify the individual species, to shed light on their individual biological functions.

Experimental

For this study, it was vital that LC-MS/MS analyses provided accurate concentrations for both C-3α and C-3β epimers, free of systematic errors. This was achieved by chemical derivatization incorporating a permanently-charged quaternary ammonium motif into the structural skeleton, which enhanced ionization and levelled response factors between epimers. Remaining problems from differential matrix suppression effects due to different retention times of the baseline-resolved epimers were compensated for by dedicated isotope standards. Compounds were measured by UHPLC and ESI-QqQ-MS in MRM mode. Serum samples of patients were obtained from a study of chronic liver diseases with various aetiologies; dried blood spot (DBS) filter cards were prepared from whole blood donor samples.

Results

Several studies have demonstrated that the C-3α epimer of 25(OH)D is present in variable concentrations in human blood, yet it is not entirely clear whether this variability is due to exogenous sources (foods, vitamin D supplements) or endogenous metabolism. Premature infants display the highest C-3α-25(OH)D levels, and hepatic immaturity has been given as one potential reason. From an analytical point of view, the C-3α epimer is a potential interference in the analytical determination of the vitamin D status marker, leading to systematic analytical errors if not properly accounted for. As the mass spectrometric properties of both epimers are very similar, separation of the two species must be achieved during HPLC separation prior to MS analysis. In the work presented here, we give a short introduction to calcaemic and non-calcaemic effects of vitamin D, in particular the differences seen for epimer species. We describe novel methods for analysis of the two epimers in serum as well as dried blood spot samples. The outcome of our research was three-fold: Firstly, we developed an assay that readily separates and accurately captures both epimer species. Simultaneously, the method provided interference-free measurement of the established vitamin D status marker. Secondly, we extended the work to analysis of dried blood spots and were able to quantitatively determine both vitamin D epimers from whole blood samples. Of note, we used a novel artificial vitamin D-free whole blood for calibration. This method is particularly interesting for analyzing infant samples, where concentrations of 3α-25(OH)D can be very high. Finally, our methods allow the individual assessment of biological effects of the epimers. As example, we investigated C-3α and C-3β 25(OH)D levels during the course of cholecalciferol supplementation in adults with chronic liver diseases.

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Excellent sensitivity through excellent recovery – ERLIC for absolute quantification of low abundant protein phosphorylation events in cancer patient tissue

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Introduction

Absolute quantification of low abundant phosphorylation events from minute amounts of sample is a prerequisite for establishing LC-MS-based phosphoprotoemics workflows in the clinics circumventing costly and time-consuming generation of site-specific antibodies. However, workflows need to exhibit excellent quantitative recovery to overcome problems with low phosphoprotein stoichiometry and the limitations of sample amount (e.g. biopsies). Here we demonstrate that Electrostatic repulsion-hydrophilic interaction chromatography (ERLIC) in comparison to the widely used TiO_2-affinity purification allows for considerably improved analyte recovery and grants unbiased access to all phosphopeptides in a digest (I). Consequently, we employed ERLIC in conjunction with targeted LC-MS for absolute quantification of low abundant protein phosphorylation events in minute amounts of tissue from colon cancer patients (II).

Methods

(I) To assess quantitative losses during enrichment (ERLIC and TiO_2), we spiked a “heavy”-labeled phosphopeptide-enriched fraction (from 100 µg) into an unlabeled-digest (100 µg) followed by another round of enrichment (2 replicates). Phosphopeptide ratios (as determined by LC-MS) reflected the quantitative recovery of each phosphopeptide.

(II) For absolute quantification of S125 phosphorylation on PHD2 (peptide: AKPPADPAAAApSPCR), 16 µg of digest from normal and cancerous colon tissue of ten patients were subjected to ERLIC (including 780 amol of a “heavy”-standard). The phosphopeptide was purified at the specific retention time followed by targeted LC-MS in parallel reaction monitoring-mode. In addition, 1.2 µg of digest (including 240 amol of a “heavy”-standard) were used for absolute quantification of the non-phosphorylated counterpart by direct LC-MS.

Results

(I) In case of TiO_2-affinity purification, quantification of 1,800 different phosphopeptides revealed an average quantitative recovery of 38 ± 2% with poor recovery rates (< 10%) for a large portion of short and basic phosphopeptides. In contrast, ERLIC demonstrated a 1.7-fold higher recovery with 65 ± 15%, as determined by quantification of 1,100 different phosphopeptides. Most notably, recovery was completely independent of physicochemical peptide properties rendering ERLIC an excellent method for efficient purification of nearly any phosphopeptide from a digest.

(II) Since antibody-based detection repeatedly failed to work, we applied an ERLIC-based targeted assay to absolutely quantify S125 phosphorylation levels of PHD2 (mediating Hif1α degradation via proline hydroxylation) in healthy and cancerous tissue of 10 colon cancer patients. PRM analysis revealed fairly stable PHD2 expression levels (358 ± 154 amol per µg protein) with phosphorylation levels of 2.5 ± 0.9% in all healthy tissue samples. Surprisingly, we detected diminished S125 phosphorylation levels in cancerous tissue of all 10 patients down to 0.9 ± 0.4% ($p \leq 0.001$), even though total PHD2 expression remained unchanged. Subsequent, biochemical validation revealed a concomitant elevation of Hif1α expression levels rendering S125 an “on/off-switch” for PHD2 activity.

Novel Aspect

Sensitivity and unbiased recovery render ERLIC an excellent tool for targeted phosphoproteomics with minute amounts of clinical tissue sample.

Identification and classification of amyloidosis by matrix-assisted laser desorption/ionization mass spectrometry imaging

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Introduction

Amyloidosis is a disease caused by extracellular accumulation of fibrillar aggregates of polypeptides. To date, 35 different peptides and proteins are known to form amyloid fibrils, thus accurate diagnosis and classification is of paramount importance to guide the patient's treatment. Currently, immunohistochemistry (IHC) is the most commonly utilized method to identify the causative protein but harbors some difficulties regarding the sensitivity and specificity. Recently, mass spectrometry-based proteomics was demonstrated to be a valuable tool to supplement the typing of amyloidosis. Although, these approaches have several advantages over IHC, there is still the need of Congo red staining to identify and/or locate amyloid deposits in the tissue section.

Methods

Formalin-fixed and paraffin-embedded tissue sections of 16 different amyloid cases including diverse amyloid types and organs were analyzed by matrix-assisted laser desorption/ionization mass spectrometry imaging (MALDI-MSI) coupled with ion mobility separation (IMS) after on-tissue tryptic digestion. Peptide identification by MSMS was performed directly on the tissue sections. A novel filter method was applied to the imaging data to reveal a universal peptide signature for amyloid deposits. The result was validated by examining a cohort of 97 cases including ALλ, ATTR amyloid cases and cases without amyloidosis. Sub-typing of the two amyloid types ALλ and ATTR was performed by a support vector machine (SVM) classification model.

Results/Discussion

Analyzing the 16 different amyloid cases by MALDI-IMS-MSI we detected tryptic peptides derived from the proteins apolipoprotein E (ApoE), serum amyloid P-component (SAP) and vitronectin (VTN) commonly present in diverse types of amyloid. Comparing the peptide images of each case with the corresponding immunostaining revealed the co-localization and specific enrichment of these peptides in amyloid deposits. Similar observations were made for peptide masses of the amyloidogenic proteins apolipoprotein AI (ApoAI), serum amyloid A (SAA) and transthyretin (TTR) in their corresponding amyloid cases. Based on these data we developed a peptide filter discriminating the peptides according to mass accuracy, drift time and an image correlation coefficient. Applying the filter on the imaging data revealed a universal peptide signature with a variable composition of peptides belonging to ApoE, SAP, VTN, whereas peptides of ApoAI, SAA and TTR can be considered as additional indicators.

These results were confirmed by examining the imaging data of the validation cohort. Furthermore, amyloid deposits were identified with high sensitivity and specificity.
Comparing the two amyloid types ALλ and ATTR, peptides derived from SAP and TTR were found more commonly for the latter. After confirmation by a Mann Whitney U test, we used these peptides to build a classification model based on a SVM algorithm. After cross validation the SVM model distinguished between the two amyloid types with high sensitivity and specificity.
Here we introduced a novel bioinformatics tool, which allows the investigation of amyloid deposits by MALDI-MSI. Furthermore, we demonstrated that MALDI-MSI can be used as an independent analytical method to assist the diagnosis and classification of amyloidosis.

PeptideMapper: Efficient and Versatile Amino Acid Sequence and Tag Mapping

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The mapping of amino acid sequences is an essential task in bioinformatics. Notably, the mapping of peptide sequences on a proteome is required for the post-processing of proteomics results. However, this step can quickly become a bottleneck when working with extensive numbers of peptides or large protein sequence databases. Here, we present PeptideMapper, a novel amino acid sequence mapper for both peptide sequences and de novo sequencing identification results. By taking advantage of the latest advances in pattern matching, PeptideMapper achieves unprecedented performance in terms of memory footprint and execution speed, with regards to both the indexing and the querying of protein sequence databases.

Experimenteller Teil

PeptideMapper is implemented in Java as part of the open source CompOmics framework [1]. For pattern matching, several fast and efficient methods (e.g. Rank queries, backward search, Huffman encoding) and lightweight data structures (i.e. FM index, wavelet tree) were utilized. Hence, searching peptides within a proteome has only a run time complexity according to the peptide length independant of the proteome length. The query function was further extended to manage amino acids of indistinguishable mass and ambiguous amino acids. Finally, the mapping of sequence tags was implemented, including PTMs.

Ergebnisse und Diskussion

The performance of PeptideMapper was evaluated on a standard desktop computer using several databases from model organisms (yeast, mouse, human) as well as a proteogenomics and a metaproteomics database. Both the indexing speed and the index size evolve linearly with the database size. In all tests, it outperforms current state-of-the-art tools, even in two orders of magnitude.

PeptideMapper is a very efficient and versatile approach for indexing entire proteomes, and is particularly well-suited for challenging experimental setups involving large databases. It has the potential to overcome several bottlenecks in proteomic data analysis workflows and is especially equipped for the handling of de novo sequencing results. It supports virtually any sequence tag, any set of PTMs, and it can quickly map large datasets onto a proteome without any cleavage restriction.

Neue Aspekte

Performance improvement and reduction of memory consumption for indexing proteomes and mapping both peptides and sequence tags.

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Comparison of Data-Independent Acquisition (DIA) and Data-Dependent Acquisition (DDA) for label-free Quantification

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In discovery-driven protein biomarker screening label-free quantification methods are increasingly used. As of now, Data-Dependent Acquisition (DDA) is the most commonly used method. For quantification purposes areas under the curves (AUC) of extracted ion chromatograms (XIC) of intact peptide precursors are calculated. Recently Data-Independent Acquisition (DIA) is being used more frequently [1]. This method fragments all peptide ions in a defined m/z interval (e.g. 20 Da). These intervals are shifted and cover entire m/z windows (spanning over several hundred m/z) within a duty cycle [2]. The identification of the resulting highly complex MSMS spectra is done using spectral libraries [3]. Quantification relies on the AUCs of the XIC of fragment ions instead of their intact precursors. Here, DIA is compared with DDA.

Experimenteller Teil

Two prostate cancer cell lines were injected subcutaneously into SCID mice. Resulting tumors were excised and prepared for LC-MSMS-analysis. For each biological triplicate data were acquired in DIA and DDA mode. For the spectral library DDA runs of each of the replicates were used.

LC-MSMS data were processed using MaxQuant (DDA quantification) and Spectronaut (DIA quantification). The spectral library was generated using Spectronaut from results using MaxQuant. Post-analysis was done using Perseus.

Ergebnisse und Diskussion

DDA and DIA datasets were compared under several different aspects. One of the main problems of quantification using DDA are missing values of peptides which are present in the sample but are not chosen by the DDA algorithm for fragmentation and therefore are not identified and as a result their AUC ignored for quantification. The aim of DIA is to reduce this problem because of the unbiased fragmentation approach. In contrast to DDA in DIA mode every peptide is fragmented. Using the generated datasets this trend is also visible with the DIA data having the higher data completeness. Other aspects that were used for comparison are the CVs, total protein identifications and reproducibility.

Using Perseus the datasets were processed and different statistical test were applied to generate lists of Proteins that were significantly regulated. These lists were then compared. Our results show that one has to expect differences when comparing these two methods. Some of these differences can be explained because of the missing values in case of DDA. Most prominent in the results is that proteins that were only identified in one cell line but not in the other were not quantified, therefore did not pass filtering and do not appear in the final result lists for DDA.

Neue Aspekte

Direct comparison of DIA and DDA label-free Quantification using non-artificial Datasets

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Differentiation of organic and conventional farming of tomatoes by non-targeted metabolomic profiling using travelling-wave ion mobility high resolution mass spectrometry

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Nowadays the appreciation of food quality and traceability are important issues to both costumers and manufacturers. The quality of food products is often linked to their origin and affects the consumer's choice looking for the quality of regional products or specialties from abroad. Both have a substantial influence on the market price of the product. Another factor causing differences in the intrinsic value of food is its way of production e.g. by organic or conventional farming of plant-derived food. Thus, to guarantee the traceability of these items from farm to fork is essential, not only for consumers but also for manufacturers and retailers. To detect food fraud in the manufacturing and supply chain specific and robust analytical methodologies are required.

In our FOODOMICS project a valid methodology for food authenticity testing by metabolomic profiling is established via liquid chromatography travelling wave ion mobility quadrupole time of flight mass spectrometry (UPLC-TW-IMS-HR-Q-ToF MS). This project is funded by the German Federal Ministry of Food and Agriculture (BMEL).

The method development was based on the commodity tomato. Here the focus was set on the differentiation of organic and conventional farming practices. Representative authentic material comprising specified stages of fruit maturity was derived from different countries of origin, comprising multiple plant varieties grown under organic and conventional farming conditions. After a QuPPe-like extraction step sample extracts were subjected to UPLC-TW-IMS-HR-Q-ToF MS in full scan $HDMS^E$ mode with ESI positive and negative polarity.

The classification of organic and conventional tomatoes was evaluated on the basis of statistical discriminative models in a metabolomic fingerprinting approach by multivariate data analysis (PCA and OPLS-DA) using EZInfo3.0 software (Umetrics Inc., Sweden) and Progenesis QI v2.2 (Nonlinear Dynamics, UK).

Subsequently targeted markers differing significantly in their abundance profiles in organically and conventionally grown fruit were selected, characterized using a metabolomic profiling workflow applying a three-point coordinate system based on the exact mass, the retention time and the collision cross section (CCS) in TW-IMS (EM_RT_CCS) and further identified due to chemical databases and reference standards. Marker compounds were classified according to their identification status and included into respective condition-specific metabolome databases. Descriptive models for classification of tomatoes from organic and conventional farming were established and validated using a blind sample approach to verify the applicability of the models in routine analysis.

Increasing arginine production in C. glutamicum by rational strain design using a combination of metabolomics and proteomics

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C. glutamicum is a bacterium used for biotechnological production of amino acids and other metabolites. Arginine is of commercial importance in cosmetic and pharmaceutical industries and as food additive.

Here we highlight that combining rational strain design with metabolomics and proteomics is a powerful tool to increase production of desired metabolites in a biotechnological workhorse.

Experimenteller Teil

Three mutant strains were compared to wildtype C. glutamicum extracts. Metabolomics and proteomics data have been acquired on an impact II QToF-MS (Bruker Daltonics). The MetaboScape software was used for processing of metabolomics data, whereas MaxQuant was used to process proteomics data. Mapping of detected changes to the arginine pathway enable data interpretation in a biological context.

Ergebnisse und Diskussion

Metabolomics and proteomics data were acquired to gain insights into changes introduced by rational strain design to increase arginine production in C. glutamicum. Metabolomics data analysis resulted in the tentative identification of an unknown compound — more abundant in the mutant strains — as glutamylvaline. Several known compounds in the arginine biosynthetic pathway could automatically be identified. Proteomics data revealed significant changes of proteins involved in the arginine biosynthesis pathway. Mapping alterations detected by both OMICS approaches on biochemical pathway maps enabled quick formulation of hypotheses for the observed changes in the biological context. Our results demonstrate that combination of non-targeted omics techniques enables in-depth investigation of changes in C. glutamicum caused by rational strain design to increase production of desired metabolites.

Neue Aspekte

Combination of non-targeted metabolomics and proteomics workflows link data to biology by pathway mapping

Application of high-throughput MS screening to disentangle the bacterial metabolome

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Introduction

Bacteria produce a wealth of structurally diverse specialized metabolites with a remarkable range of activity. Recently augmented knowledge about bacterial genomes has revealed that many bacteria have far greater potential to produce secondary metabolites. This potential, however, has been hampered by difficulties in metabolite extraction or non-expression of genes. Many microbial gene clusters may be silent under standard laboratory growth conditions. One promising approach to trigger the activation of cryptic biosynthetic pathways is the co-cultivation of two or more microorganisms in the same confined environment, leading to the production of new metabolites. Because of the complexity of microbial extracts, advanced analytical methods are key for the successful detection and identification of co-culture-induced metabolites.

Experimental

In the present study, the secondary metabolites produced by 12 phylogenetically different bacteria isolated from soil and rhizosphere were analysed. Liquid Extraction Surface Analysis (LESA) combined with a Thermo Scientific LTQ Orbitrap XL mass spectrometer was applied using various solvents. The bacteria were also selectively cocultured and grown under three different nutrient conditions namely, nutrient-rich 1/10 TSBA; nutrient-poor Water Agar and Water Agar supplemented with Artificial Root Exudates. Full scan mass spectra were generated using 30,000 m/Δm resolving power. PCA was performed on the full-scan data of the samples using Metaboanalyst 3.0, a web-based tool for metabolomic data processing, statistical analysis, and functional interpretation.

Results and discussion

Our results revealed that LESA with high-resolution MS is a powerful tool for high-throughput extraction and detection of secondary metabolites produced by different bacteria under different culture conditions. Of all the solvents tested, ethyl acetate/acetone (65:35, v/v) containing 0.1% formic acid revealed the most effective extraction. Pyrrolnitrin, a chlorinated phenylpyrrol antibiotic was detected in *Serratia plymuthica* on nutrient-rich 1/10 TSBA and

Water Agar supplemented with Artificial Root Exudates but not on nutrient-poor Water Agar. A violet pigment, violacein, and indole-3-carboxaldehyde, both indole-derived antibiotics were detected in *Janthinobacterium sp*. AD80 only under nutrient-rich growth condition. Bioactive molecules Pseudopyronin A & B and Pyocyanin in *Pseudomonas sp*. were also identified. Besides known secondary metabolites, several unknown metabolites were detected in bacterial cultures but not in any of the controls consisting of only media.

Novel Aspect

LESA-HRMS is a fast, sensitive and cost-effective high-throughput screening device for direct detection of bacterial secondary metabolites produced under different cultures conditions.

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Keywords

LESA-HRMS, microbial co-cultures, rhizosphere

The Next Generation Ion Mobility Separation (IMS) Adds A New Dimension to Substance Characterization and Identification

Detlev Suckau, Sven Mayer, Verena Tellström

Introduction

Substance characterization by mass spectrometry typically involves the dimensions of MS and MS/MS analysis. Current high resolution QTOF instruments add the dimensions of true representation of isotopic patterns of precursor as well as the fragment ions, which enhance the capability of determining a compounds and its subunits element formula significantly.
In this work we utilize the timsTOF ion mobility QTOF instrument to further enhance the analytical options beyond those 4 dimensions for compounds that are otherwise difficult to separate and to analyze, such as carbohydrate, flavonoid or lipid isomer analysis. Ion mobility separations on timsTOF can be scaled with regards to the analysis scope and reaches mobility resolutions beyond 200.

Experimental

Lipids, oligosaccharides and flavonoids were purchased, propolis samples were obtained from bee hives by SM. Lipid samples were 18:1 Δ9-cis PC and 18:1 Δ6-cis PC, as well as 16:0-18:0 PC, 16:0-18:1 PC and 16:0-18:2 PC, and trisaccharides (raffinose, melezitose and maltotriose. The ability to separate isomers as well as lipids with partially overlapping isotopic distributions was investigated using IMS and to obtain MS and MS/MS spectra without interference. All spectra were obtained from infusion or LC-IMS-QTOF MS and MS/MS analysis on a Bruker timsTOF with trapped IMS (TIMS) funnel. The ions were trapped, ramped electric field gradients were used to release the ions according to their mobility in a constant gas flow.

Results

Several mixtures of isomeric compounds of different structural classes were investigated. Several of the isomeric compounds showed very similar or identical retention times in standard screening LC-gradients. This complicated the interpretation of MS and MS/MS spectra in standard analyses of lipids or flavonoids such as quercetin or morin. In the case of lipid analysis, the interpretation of fragment spectra is further hampered by partially overlapping isotopic patterns of lipids with one additional or fewer double bonds. Here, the additional dimension of ion mobility helped to obtain clean MS and MS/MS spectra for compound characterization. All isobaric compounds could be baseline separated in the mobility domain. IMS resolving powers were obtained in the range between 100-250. From the 1/k0 mobility values, the collision cross section (CCS) values were calculated and compared to published values. The fragment spectra after mobility separation were evaluated as well as their isotopic pattern qualities. For lipid analysis the mobility separation simplified their identification due to clean isotopic patterns of fragment peaks.

Several of the isomeric flavonoids co-eluted from column. Using an MS acquisition speed of 2 Hz and a mobility ramp time of 140 µs, the isobaric compounds could be base line separated in the mobility domain at LC peak widths of around 10 s. This demonstrates the general usability of trapped IM-MS in complex metabolomics studies like shown for the plant flavonoids.

TIMS introduces a new dimension of molecular separation and characterization, which significantly extends the capabilities of current high resolution mass spectrometry platforms. The value added by the ion mobility separation dimension for the identification of isomers or homologues was found significant.

New Findings

TIMS yields mobility separations in excess of 200 adding a new dimension to isomer identification in LC-IMS-MS and MS/MS workflows.

Keywords

QTOF, ion mobility, CCS, isomers, lipids, flavonoids

Cytochrome c-mediated modification of cardiolipin

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The small heme protein cytochrome c (cyt c) has important functions as redox carrier in the mitochondrial electron-transport chain. In the intermembrane space of mitochondria cyt c is closely associated with the unique phospholipid cardiolipin. Upon release from stressed mitochondria this protein is also involved in apoptosis induction. However, in functioning mitochondria the physiological significance of alterations in cyt c-cardiolipin interaction remains largely unknown. Own studies have demonstrated an iron release from cyt c by hydrogen peroxide and "Fenton-like" lipid modifications in cardiolipin-containing liposomes. By using HPTLC and MALDI-TOF MS we could identify the products of free radical transformations occurring in the polar region, as well as in the fatty acid chains of cardiolipin.

Experimenteller Teil

The solvents, MALDI matrixes (9-aminoacridine, 2,5-dihydroxybenzoic acid) as well as primuline, horse heart cyt c, hydrogen peroxide, ascorbic acid and glutathione were obtained from Sigma-Aldrich in the highest commercially available quality and used without purification. All phospholipids were obtained from Avanti Polar Lipids.

Large unilamellar vesicles composed of tetraoleoylcardiolipin (TOCL) and dioleoylphosphatidylcholine (DOPC) (1:1 molar ratio) were formed by using the extrusion technique.

High-performance thin layer chromatography (HPTLC) plates (silica gel H 60, thickness - 0.3mm, Merck, Darmstadt, Germany) have been used to study the lipid transformations. Lipids were extracted from the gel and spotted on the MALDI plate along with the matrix. All MALDI-TOF mass spectra were acquired on a Bruker Daltonics workstation (Bruker Daltonik GmbH, Germany).

Ergebnisse und Diskussion

To mimic stress conditions in mitochondria, unilamellar liposomes containing cardiolipin were exposed to hydrogen peroxide in the presence of reducing agents like ascorbic acid and glutathione. Afterwards, lipids were extracted and separated by HPTLC, visualised by primuline and subjected to MALDI-TOF MS analysis. We could show that cardiolipin facilitates the release of heme iron from cyt c upon interaction with hydrogen peroxide. This free iron can participate in Fenton-like mechanism inducing free radical modifications of cardiolipin.

In the system containing ascorbic acid or glutathione we could identify products of cardiolipin polar head fragmentation phosphatidic acid and phosphatidylhydroxyacetone. Additionally, cardiolipin aldehydes, lyso-cardiolipin and lyso-cardiolipin aldehydes have been identified. These products have not been described before in cyt c – cardiolipin interaction.

Cardiolipin species with hydroperoxide moieties in the alkyl region are a well-studied product of cyt c-cardiolipin interaction. These products are involved in cyt c release into cytoplasm and apoptosis induction [1]. The other known process of cyt c-mediated damage is free radical fragmentation of the cardiolipin polar head [2]. Cardiolipin polar head fragmentation yields to the formation of phosphatidic acid and phosphatidylhydroxyacetone [3]. Phosphatidic acid is a second messenger in cells, as it was shown to interact with the mTOR pathway. Being synthesized in the outer mitochondrial membrane by mitochondrial phospholipase D (mPLD) phosphatidic acid is also involved in the process of mitochondrial fusion.

From our data, we can conclude that, the interaction of cyt c with cardiolipin in the presence of hydrogen peroxide leads to a variety of cardiolipin degradation products, some of them haven't been observed before. By these mechanisms, the integrity of mitochondrial membrane will be disturbed and the apoptosis of cells will be induced.

Neue Aspekte

The formation of lyso- and aldehyde- cardiolipin via interaction with cyt c, hydrogen peroxide and glutathione has been observed.

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A new bridge between targeted and non-targeted LC-MS/MS lipidomics

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Skyline, a powerful software primarily designed for proteomics applications, was successfully extended to targeted LC-MS/MS lipidomics [1, 2]. This proof-of-principle study provided a systematic workflow for the straightforward method design and analysis of selected reaction monitoring (SRM) data in lipidomics based on lipid building blocks. To strengthen the LC-MS/MS lipidomics workflow and to provide a user-friendly interface for lipid researchers, we developed a native tool named "LipidCreator" which has several features including i) using lipid building blocks, ii) latest lipid nomenclature, iii) lipid fragmentation, iv) transition mass-calculator, v) spectral library generator and vi) the direct communication with Skyline.

Experimenteller Teil

Experimental section

Two proof of concept studies were conducted to the peptide system of Skyline. The first study was to use tailored modifications to create pseudo peptide sequence representing lipid species. Afterwards these pseudo sequences were adapted to the proteomics workflow in Skyline. The second study was a data independent acquisition (DIA) analysis with in-silico spectral library. The library was generated and used for matching lipids data from DIA. Furthermore, the in-house tool LipidCreator was developed to promote lipidomics in Skyline. LipidCreator was written in C#, which is compatible with Skyline. The pre-defined fragmentation in LipidCreator for each lipid class was obtained from synthetic lipid standard and analyzed with high-resolution MS.

Ergebnisse und Diskussion

Results and discussion

The results of proof of concept studies indicated that Skyline has great potential to work with both targeted and non-targeted lipidomics. To enhance the LC-MS/MS based lipidomics workflow, we developed the in-house tool LipidCreator to generate transition lists and spectral libraries to work in Skyline. Since Skyline is a vendor independent platform, it supports SRM data from triple quadrupole mass spectrometry and parallel reaction monitoring (PRM) data from Orbitrap high resolution mass spectrometry for interpretation and visualization. PRM data evaluation is different from SRM because PRM generates MS2 spectra which require a library for comparison. Thus, we established an in-silico spectral library computing system for lipid species by computing fragments from known lipid fragmentation patterns in LipidCreator. This in-silico spectral library computing system is not only used for PRM data inspection but also will be the foundation for further data independent acquisition (DIA) analyses.

Neue Aspekte

Novel aspects

In-house tool LipidCreator bridges the gap between targeted and non-targeted LC-MS/MS lipidomics.

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Lipidomes of human lung tissues show distinct lipid metabolic alterations for lung cancer and pulmonary emphysema

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Introduction

Lipids play a crucial role in the function of mammalian lungs. As components of the pulmonary surfactant lipids stabilize the alveoli and maintain immune regulative functions. To date, little is known about the lung lipidome and its alterations in lung cancer and chronic obstructive pulmonary disease (COPD).

Previous studies showed lipidome alterations in COPD[1]. Associations between lipid metabolism and histologic phenotypes of COPD, like emphysema, are poorly understood. Emphysema is a pathologic enlargement of alveoli often occurring in COPD. Our study describes the lipidome of human lung tissue and its modulation in context of histologic phenotypes and clinical parameters.

Methods

Tumor-containing and tumor-free alveolar lung tissue biopsies were taken after surgical tumor removal from lung cancer patients. Each biopsy was processed separately for histopathological analysis and lipidomics.

Histologic phenotypes were described by a tissue specific scoring system comprising emphysema, inflammation, fibrosis and alveolar macrophages for alveolar tissues and relative proportions of vital tumor, necrosis and stroma for tumor-containing tissues.

Shotgun lipidomics[2] was performed after tissue homogenization and lipid extraction[3]. We used an Apex Qe FT-ICR-MS (Bruker) and a Q Exactive Plus (Thermo) equipped with the TriVersa Nanomate (Advion) nanoESI-source. Lipid identification was performed with LipidXplorer[4]. PCA and hierarchical clustering were used for data analysis. Partial least squares regression (PLSR) was applied to associate histopathology and lipidomics.

Results and Discussion

Lipidomes of tumor-free and tumor–containing lung tissues had distinctive alterations suitable for tissue discrimination. Tumors were characterized by high proportions of neutral lipids like triacylglycerols (TAG) and cholesterol esters (CE) as well as reduced abundances of surfactant related lipids like saturated phosphatidylcholines (PC) and phosphatidylglycerols (PG) when compared to the alveolar controls.

Hierarchical cluster analysis revealed that most types of Non-Small-Cell-Lung-Cancer, including adenocarcinomas (ADC) and squamous-cell carcinomas (SCC), had comparable lipid profiles. However, a separated branch for carcinoid lung tumors was observed indicating specific lipid metabolic alterations. We further investigated if ADCs and SCCs could be differentiated by their lipidomes. We were able to define a lipid score that discriminated both with high specificity. In the next step, lipidome data were associated to histopathological scores. We found that relative proportions of stroma, vital tumor and necrosis are most influencing factors on the tumor lipidome.

In general, tumor-free alveolar tissues were characterized by high abundances of known components of the pulmonary surfactant. Nevertheless, hierarchical clustering showed sub-clusters with lower proportions of PG and high amounts of TAG. Lipidomes of alveolar lung tissues were found to be influenced by the pulmonary emphysema and also by aging; two factors that could potentially be connected[5].

Recently, we started a follow-up study comprising tissues of 170 patients specifically focusing on lipidome alterations occurring during development of emphysema and aging. For that, we employed an advanced acquisition strategy, where overlapping *m/z* windows with a width of 150 Da were combined for the complete MS1 spectra ranging from *m/z* 300 to 1200. We observed improved quantification and recovery for low abundant species. Overall robustness of quantitative lipid profiles was improved allowing in-depth analysis of lipid metabolic perturbations.

New Aspects

This is the first study combining histopathology with shotgun lipidomics and showing distinct lipidome alterations in lung cancer and emphysema.

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Keywords

Lung tissue, emphysema, lipidomics, histopathology, multivariate statistics

Topic: Lipide & Lipidomics

Untersuchungen zu den unimolekularen und stoßaktivierten Fragmentierungsmechanismen der Diethyltoluidine über Isotopenmarkierungen

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Einleitung

Das Diethylanilin zeigt nach Elektronenionisation die literaturbekannten Verluste von 15 Da und 43 Da [1]. Untersuchungen mit *Mass-Analyzed-Ion-Kinetic-Energy*-(MIKE)-Spektrometrie zeigen dabei, dass sich der Verlust von 43 Da aus dem sequenziellen Verlust von 15 Da (Methylradikal) und 28 Da (Ethen) zusammensetzt.

Diethyltoluidine unterscheiden sich vom Diethylanilin nur durch eine Methylsubstitution am aromatischen System und zeigen neben den literaturbekannten Verlusten weitere Fragmente in den MIKE-Spektren der $[M\text{-Methyl}]^+$-Vorläuferionen. Unter unimolekularen Fragmentierungsbedingungen wird hier der zusätzliche Verlust eines Methylradikals beobachtet, unter Stoßbedingungen treten zusätzlich Verluste von 16 Da (Methan) und 30 Da (Ethan) auf. Die Intensität dieser Signale ist abhängig von der Substitutionsposition der Methylgruppe.

Die Mechanismen der zugehörigen Fragmentierungen sind noch nicht eindeutig bestimmt. Um weitere Hinweise zu erhalten, wurden vielfältige Isotopenmarkierungsexperimente durchgeführt.

Experimenteller Teil

Es wurden die drei Isomere des Diethyltoluidins untersucht. Zusätzlich wurden verschiedene Isotopenmarkierungen (Deuterium und ^{13}Kohlenstoff) an den Diethylaminoseitengruppen der Moleküle vorgenommen.

Alle Messungen wurden mit einem Micromass ZAB-2F der Firma Vacuum Generators durchgeführt. Die Proben wurden in die Gasphase überführt und mittels Elektronenionisation ionisiert. MIKE-Spektrometrie der gebildeten Ionen lieferte Informationen über die Fragmentierungsreaktionen und Werte für den *Kinetic Energy Release* (KER). Es wurden Messungen ohne Stoßaktivierung und mit Stoßaktivierung im zweiten feldfreien Raum durchgeführt. Als Stoßgas wurde Argon verwendet.

Ergebnisse und Diskussion

Alle untersuchten Verbindungen zeigten nach Elektronenionisation in den MIKE-Spektren der $M^{+\bullet}$ nur den Verlust eines Methylradikals. Dieses Verhalten trat dabei unabhängig von der

Stoßaktivierung und der Position des Methylsubstituenten am aromatischen System auf. Mit Deuterierungsexperimenten konnte belegt werden, dass die Fragmentierung ausschließlich an der Diethylaminoseitengruppe stattfindet.
In den MIKE-Spektren der $[M\text{-Methyl}]^+$ traten für alle drei Isomere unter unimolekularen Bedingungen nur zwei Fragmente auf. Über ^{13}C-Isotopenmarkierung konnte der Verlust von Ethen eindeutig als reiner Verlust aus der Diethylaminoseitengruppe identifiziert werden. Zusätzlich konnten mindestens drei unterschiedliche Mechanismen für den Verlust des Methylradikals gefunden werden, die in unterschiedlicher Häufigkeit zur Bildung des Fragments beitragen. Für dieses Fragment zeigt sich ein starker *ortho*-Effekt. Dadurch kam es zu einem Auswaschen der Deuteriumlabel aller markierten Diethyl-*o*-toluidine, das bei den anderen beiden Isomeren nicht auftrat.
Unter stoßaktivierten Fragmentierungsbedingungen war der Verlust von Methan nur für das o-Isomer zu beobachten. Über Deuterium- und ^{13}C-Markierungen ließ sich der Verlust mit hoher Wahrscheinlichkeit dem Verlust einer Methylgruppe aus der Diethylaminoseitengruppe und einem Wasserstoffatom der Ringmethylgruppe zuordnen.
Der bei allen Isomeren unter Stoßaktivierung auftretende Verlust von Ethan konnte über zwei Mechanismen erklärt werden. Eine Möglichkeit war dabei ein konzertierter Mechanismus mit sechsgliedrigem Übergangszustand, der nur für *ortho*-Isomere möglich ist. Die andere Möglichkeit war ein zweistufiger, radikalischer Mechanismus, bei dem zwei Methylradikale abgespalten werden.

Neue Aspekte

Es wurden mögliche Mechanismen für die Fragmentierung von Diethyltoluidinen vorgeschlagen und mittels Isotopenmarkierungen näher untersucht.

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Stichworte

Fragmentierung

Fragmentierungsmechanismen

Anilinderivate

Isotopenmarkierung

Stoßaktivierung

One-electron reduction of isolated metallo-supramolecular aggregates

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Are the metal centres in metallo-supramolecular aggregates electronically isolated from each other? Is there an information transfer via ligands or space? How redox-innocent are the ligands? Gaining knowledge on the redox behaviour of metallo-supramolecular aggregates in solution is highly desirable, but rather difficult due to the inherent lability of the system: It is hard to oxidise or reduce only the aggregate of interest – and not affect one of the other compounds of the (desired) manifold of species present in equilibrium. Herein, a means is presented to study the reduction of isolated supramolecular aggregates under well-defined conditions using mass-spectrometry.

During ETD and ECD, a single electron is attached to the metallo-supramolecular aggregate. The resulting reduced species is either characterised by high resolution tandem mass-spectrometry or can even be subjected to another reducing step (ECD/ECD) prior to analysis. The presented examples include the stepwise reduction of a copper(II) helicate reveiling otherwise unaccessible mechanistic details of its interconversion to the respective copper(I) congener with different stoichiometry.[1] Single-electron reduction of homoleptic metallosupramolecular squares shows the non-innocence of bipyridine ligands [2] whereas a similar experiment with bimetallic squares [3] enables the differentiation between different reduction sites. The effect of linker length is illustrated by reduction of dinuclear gold macrocycles of various ring sizes.[4]

Experimental

High-resolution electrospray ionisation (ESI) mass spectra were recorded on a Bruker Apex IV FT-ICR or a Thermo Fisher Scientific LTQ Orbitrap XL mass spectrometer. A series of multiply charged cations typically is observed for metallo-supramolecular aggregates due to abstraction of several anions during the ESI process. After mass-selection of the species of interest, one-electron reduction is performed in the gas phase using the electron capture dissociation (ECD) technique in the FT-ICR or the electron transfer dissociation (ETD) method in the ion trap module of the Orbitrap XL instrument. Reduction products of interest were again isolated and fragmented by collision-induced dissociation (CID) or subjected to a second one-electron reduction step.

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Formate attachment to ZnPorphyrin- and ZnPhthalocyanine-Oligomers: Binding, Fragmentation, Affinity.

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Introduction:

Metallated Porphyrins (Por) and Phthalocyanines (Pc), e.g. ZnPor and ZnPc, are ionized during negative ion-mode electrospray ionization (ESI) by the attachment of a formate anion to the metal center.[1] Under collision-induced dissociation (CID) conditions the complex composed of one macrocycle and one formate anion undergoes CO_2-loss yielding the hydride anion. As a consecutive fragmentation hydrogen-loss is observed, due to charge transfer from the hydride to the macrocycle, producing its true molecular anion radical.[1] Comparison of Porphyrin- and Phthalocyanine-oligomers reveals significant differences in their interactions with the formate anion. This study focuses on these differences in formate binding of ZnPor- vs. ZnPc-oligomers, as well as their fragmentation behavior. Furthermore, the relative formate anion affinity is investigated by the kinetic method.

Experimental:

ESI-MS and -MS/MS experiments were performed using a quadrupole time-of-flight instrument (QqToF) (micrOTOF QII, Bruker Daltonics, Germany). The synthesis of the target molecules were published recently. [2,3]

Results:

Covalently linked dimers of either zinc-porphyrins (ZnPor) or zinc-phthalocyanines (ZnPc) were investigated by ESI-qToF MS. The linker, connecting two macrocycles, is a flexible organic chain and can be further functionalized with a central C_{60}, resulting in four different molecules, including the dimers $(ZnPor)_2$ and $(ZnPc)_2$ as well as $(ZnPc)_2C_{60}$ and $(ZnPor)_2C_{60}$. The ion formation by formate anion attachment to the four

different molecules was investigated, together with the fragmentation behavior of the resulting adduct anions.

$(ZnPor)_2$ binds exclusively only one formate anion, without any sign of a doubly anionized species, from which we assume the formation of a sandwich-like adduct. $(ZnPor)_2C_{60}$, however, displays in addition to the $M+HCOO^-$ peak also a species with two formates attached to it. Therefore, the C_{60} is now most likely sandwiched by the two ZnPor units to enable formate binding to the two zinc-centers on the outside. In case of the $(ZnPc)_2$ dimer the fullerene moiety is not required to form dianions, as signals for the attachment of one and two formate anions are observed, indicating a higher formate affinity of the ZnPcs compared to the ZnPors.

The CID behavior of the doubly anionized adducts of $(ZnPor)_2C_{60}$ and $(ZnPc)_2C_{60}$ affirms this assumption: the porphyrin species fragments solely by loss of a charge carrier ($-HCOO^-$) turning into a monoanion, whereas the phthalocyanine additionally loses CO_2 remaining a doubly charged species. Further CID losses of H/CO_2 lead eventually to a truly uncommon species, i.e. the true molecular dianion of $(ZnPc)_2C_{60}$.

The relative affinity was also studied by Cooks' kinetic method. Common ZnPor and ZnPc monomers were mixed together with formate anions. CID of the formate-bound heterodimers showed only signals with ZnPc retaining the formate anion.

New aspects:

Differences in anion binding between ZnPors and ZnPcs and their relative formate affinities. Formation of true molecular dianions.

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Topic:

Gas-phase reactions & fragmentation

Keywords:

Formate attachment, ZnPorphyrin, ZnPhthalocyanine, true molecular dianions

Category:

Zinc-Porphyrins/Phthalocyanines

REACTIVITY AND STABILITY CHECK OF EVEN VS. ODD ELECTRON (QUASI)-MOLECULAR IONS DERIVED FROM TRIANGULENIUM TYPE DERIVATIVES

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Introduction

Triangulenes are characterized by six six-membered mostly carbon-based rings fused in a triangular, planar fashion. The name is nowadays used for a diverse class of molecules with a variety of central atoms, functionalizations, bridging modes and ring openings with a vast range of applications from bioimaging to physisorption of CO_2.
The present work represents the first mass spectrometry-based investigation of this class of compounds. Nitrogen-centred triangulene derivatives, which could be produced as odd-(OE) and even-electron (EE) ions allowed investigation of their stability towards collision-induced dissociation (CID). The second study included carbenium ion-centered triangulenes with peripheral tertiary amines. The dissociation behaviour of these EE molecular ions is influenced by their electronic (odd vs. even electron) and molecular structure (planar vs. non-planar).

Experimental

Electrospray ionization (ESI) experiments were conducted with a quadrupole time-of-flight mass spectrometer (micrOTOF-Q II, Bruker) with support (MS^3, MS^4) from a quadrupole ion trap (esquire6000, Bruker) and a FT-ICR (SolariX XR 12R, Bruker) instrument. The heterotriangulenes were separately dissolved in acetonitrile and diluted with DCM/ACN=1:2 and DCM/MeOH=1:2. The resulting solutions were introduced into the ESI ion source by direct infusion.

Results and Discussion

N-centered triangulenes:
A series of dimethylmethylene-bridged triangulenes with a central nitrogen atom and decorated with 0 to 3 electron-withdrawing 4-pyridyl groups is studied by ESI. Ion formation occurs by two competing pathways: oxidation and/or protonation of one of the pyridyl groups. With increasing number of pyridyl groups, the probability of protonation increases while radical-cation formation becomes less pronounced. However, it is possible to generate OE and EE ions from the same molecule. Thus, these molecules represent text book-like candidates to

study the stability of OE vs. EE ionic structures of the same molecule. This is done in energy-dependent CID experiments. Both systems exhibit the same fragmentation behaviour, however, the OE radical cation shows considerably less stability compared to the EE protonated molecule. The radical cation forms a fragment ion with an extended aromatic system that is energetically favoured, facilitating fragmentation. Ab initio and density functional theory calculations support this interpretation.[1]

Carbenium-centred triangulenes:
Triangulenic derivatives with central carbenium ions are truly pre-formed organic ions, which can be directly transferred into the gas phase without ionization step. Thus, a cationic EE precursor for fragmentation is obtained. The EE precursor fragments by release of an alkene, retaining its EE character, obeying the “even-electron rule”. However, it also shows abundant loss of an alkyl radical, forming OE systems and contradicting the “even-electron rule”! We explain the formation of OE fragment ions by sufficient stabilization due to the large π-system. The beauty of this system is concurrent formation of EE and OE product ions which allow the study of the fragmentation behaviour as a function of the electronic nature of the same molecular framework. This enables us to draw a detailed mechanistic path for the ions, which reveals that reactivity is influenced by both their electronic nature and molecular structure.[2]

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Novel aspects
First mass spectrometry-based investigation of triangulenes with emphasis on the distinct OE and EE ion stability in energy-dependent CID.

Dissociation behavior of a TEMPO-benzyl cross-linker for peptide structure analysis by free radical initiated peptide sequencing (FRIPS) mass spectrometry in negative ESI-MS

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Introduction

We synthesized a cross-linker containing a TEMPO (2,2,6,6-tetramethylpiperidine-1-oxy) moiety connected to a benzyl (Bz) group , termed TEMPO-Bz-linker.[1] The aim for designing this novel cross-linker was to facilitate MS analysis of cross-linked products by free radical initiated peptide sequencing (FRIPS)[2] and to evaluate the potential of the TEMPO-Bz-linker for protein 3D-structure analysis. Previous (+)-ESI-MS/MS studies had revealed an unexpected fragmentation behavior of the TEMPO-Bz-linker upon collisional activation following two distinct fragmentation pathways, depending on charge state and amino acid sequence of the peptides involved.[1, 3] (-)-ESI-MS, MS/MS, and MS^3 experiments of cross-linked peptides allowed elucidating the fragmentation behavior of deprotonated TEMPO-Bz species.[4]

Methods

Angiotensin II and ACTH (fragment 18-39) were purchased from Sigma-Aldrich, test peptide 1 (Ac-TRTESTDIKRASSREADYLINKER) was obtained from Creative Molecules Inc. The TEMPO-Bz-linker (1 mM in DMSO) was added to the peptide solution in 20 mM HEPES, pH 8.5 (cross-linker/peptide ratio 1:1). The reaction was allowed to proceed at 25°C for 2 hours before cross-linked test peptide 1 was digested with trypsin. All other crosslinked peptides were used directly. (-)-ESI-MS, MS/MS, and MS^3 analyses were performed on an Orbitrap Fusion mass spectrometer (Thermo Fisher Scientific). For MS/MS measurements, ions were isolated in the quadrupole, fragmented by CID and analyzed in the orbitrap mass analyzer (R = 120,000 at *m/z* 200).

Results and Discussion

Cross-linking of three model peptides (angiotensin II, ACTH, and test peptide 1 (Ac-TRTESTDIKRASSREADYLINKER)) was performed with our novel MS/MS cleavable TEMPO-Bz-linker. For elucidating the fragmentation behavior of the cross-linker, (-)-ESI-CID-MS/MS and MS^3 experiments were performed. Data analysis was performed with the in-house software MeroX [5] and by manual assignment of FRIPS fragments and neutral losses. (-)-ESI-MS^3 spectra were collected to examine the different fragmentation behavior of TEMPO- and Bz-modified peptide chains. Side-chain fragmentation was preferentially observed for Bz-modified peptides, while backbone fragmentation was dominant for TEMPO-modification. The cross-linked, 3- charged precursor ion of test peptide 1 fragmented homolytically, as expected, at the NO-C bond of the TEMPO-Bz-linker. (-)-ESI-MS/MS indicated a high degree of backbone fragmentation of peptides (a, x, c, y-type ions). Also, the 2- charged precursor ion of two intermolecularly cross-linked angiotensin II molecules showed the expected homolytic fragmentation of the TEMPO-Bz-linker. Assigning all fragment ions in (-)-ESI-MS, MS/MS, and MS^3 was challenging due to the complex fragmentation pathways of TEMPO-Bz-crosslinked peptides. We show that the TEMPO-Bz-linker is highly beneficial for conducting FRIPS in negative ionization mode as the desired homolytic cleavage of the NO-C bond is the major fragmentation pathway. Based on characteristic fragments, the isomeric amino acids leucine and isoleucine could be discriminated. Interestingly, we observed pronounced amino acid side chain losses in cross-linked peptides if the cross-linked peptides contain a high number of acidic amino acids.

New Aspects:

The novel TEMPO-Bz-linker is applicable for FRIPS in negative ion mode as the desired homolytic cleavage of the NO-C bond is observed.

Keywords

(-)-ESI-MS, peptide cross-linking, free radical-initiated peptide sequencing, TEMPO-Bz-linker, CID-cleavable cross-linker

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- Titel

Online SPE-HILIC-ESI-MS/MS zur Untersuchung des Metabolismus von auf Acetyl-CoA und Malonyl-CoA in MCF-7 Brustkrebszellen

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- Einleitung (max. 120 Wörter)

Coenzym A besteht aus ATP, Pantothenat (Vitamin B5) sowie Cysteamin und wird im Metabolismus mit Carbonsäuren zu Acyl-CoAs umgesetzt. Acetyl-CoA ist das wichtigste Derivat und spielt in verschiedenen Stoffwechselwegen wie zum Beispiel der Glykolyse oder dem Citratzyklus eine wichtige Rolle. Acetyl-CoA ist zudem Vorläufer für Malonyl-CoA, welches Ausgangsstoff in der Fettsäuresynthese ist. Acetyl-CoA-Carboxylase katalysiert die Reaktion von Acetyl- zu Malonyl-CoA, kann aber durch die Substanz 5-Tetradecyloxy-2-furancarbonsäure (TOFA) inhibiert werden. Die Kontrolle der Fettsäuresynthese und damit auch der Malonyl-CoA Synthese spielt eine wichtige Rolle in Brustkrebszellen der Linie MCF-7. Durch die Abnahme der Fettsäuresynthese sinkt die Zytotoxizität sowie die Apoptoserate.[1]

- Experimenteller Teil (max. 120 Wörter)

Für die Coenzym A Derivate Acetyl- und Malonyl-CoA konnte mithilfe einer Amid-HILIC Phase erfolgreich eine chromatographische Trennung entwickelt werden. Diese zeigte Nachteile beim Einsatz mit Realproben, weshalb ein zusätzlicher Probenvorbereitungsschritt integriert werden musste. Die online SPE bietet die Möglichkeit den Aufarbeitungsschritt in die bestehende chromatographische Methode zu integrieren und automatisiert ablaufen zu lassen. Mithilfe eines schwachen Anionenaustauschers war es möglich die sehr polaren und anionischen CoA Derivate auf der stationären Phase zu retardieren und anschließend wieder zu eluieren.

Die Effekte für die Verbesserung und der möglichen Ionensuppression wurden mit Hilfe eines Nachsäuleneintrags von d_3-Hydroxyy-methyl-glutaryl-CoA untersucht. Um Matrixeffekte zu

bestimmen wurden die Realproben sowohl mit als auch ohne online SPE im hochaufgelösten Full Scan an einem Orbitrap-MS analysiert.

- Ergebnisse und Diskussion (max. 300 Wörter)

Aufgrund der intrazellulären Konzentration im Spurenbereich ist eine sensitive analytische Methode zur Quantifizierung notwendig. Durch die noch nicht weit verbreitete Kombination von online-Festphasenextraktion (SPE) mit der Hydrophilen Interaktions-Flüssig-Chromatographie (HILIC) war es möglich, den Probenvorbereitungsschritt in die chromatographische Trennung zu integrieren. Mithilfe eines Triple-Quadrupol Massenspektrometers im MRM-Modus nach positiver Elektrospray-Ionisierung konnte sensitiv detektiert und quantifiziert werden. Dabei konnten Bestimmungsgrenzen zwischen 1 nM und 5 nM bzw. Nachweisgrenzen zwischen 2,5 nM und 10 nM ermittelt werden. Es konnte weiterhin gezeigt werden, dass mithilfe der online-SPE nicht nur Zeit eingespart werden kann, sondern die entwickelte Methode chromatographische Vorteile und geringere Matrixeffekte gegenüber der reinen HILIC Methode aufweist.

Nach erfolgter Methodenentwicklung mit Standards war es möglich die Anwendbarkeit der Methode am Beispiel von MCF-7 Zellen zu demonstrieren. Es konnte zudem gezeigt werden, dass sich das Acetyl-CoA zu Malonyl-CoA-Verhältnis durch Einsatz von TOFA im Vergleich zur Kontrollprobe deutlich verschiebt.

- Neue Aspekte (max. 20 Wörter)

HILIC-MS/MS zur Analyse von Coenzym A Derivaten mit online Probenvorbereitung

- Referenzen (max. 5)

[1] Ellen S. Pizer, Jagan Thurapi, Wan Fang Han, et al. *Cancer Research* **2000**, *60*, 213-218.

- Stichworte (max. 5)

online-SPE-HILIC, Coenzym A Derivate, MS/MS,

LC/MS²-standards library using high-resolution accurate mass (HRAM) platform for metabolomics research

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Introduction

Metabolite identification is an increasing challenge in untargeted LC/MS metabolomics studies. For unambiguous metabolite identification, high mass accuracy, high-quality fragmentation spectra and retention times under specific liquid chromatographic conditions are essential. Although, there are several libraries available to address these needs, they suffer some limitation. In particular, the quality of the MS^2 spectra at different collision energies are not manually curated, the mass accuracy and resolution at MS^1 and MS^2 are not consistent and most of the MS spectra in those libraries are not generated using pure synthetic standards. Moreover, there are no libraries of retention times at different liquid chromatographic conditions. Therefore, an LC/MS^2 library of high resolution and accurate mass spectra are warranted.

Experimental

We used a library of pure synthetic standards of > 600 metabolites covering most of the metabolic pathways. A flow injection/SIM/ddMS^2 method was developed to generate the MS^2-spectra in positive and negative mode. Every standard was injected separately using the flow injection method. Selected ion monitoring followed by data-dependent MS^2 scans were performed at different collision energies using a hybrid quadrupole-Orbitrap mass spectrometer (Q-Exactive). For the metabolites that had good MS^2 spectra, several LC conditions were used to develop the LC library. 12 different LC columns covering most of the commercially available column chemistries, different flow rates, gradients, solvents and injection volumes solvents were used. Data analysis was performed by using FreeStyle, Library Manager and Tracefinder.

Results

We developed a method to automatically acquire MS^2 spectra at different collision energies without the need for manual injection. Data-dependent acquisition of the pure standard proved superior to other scan modes on the Q-Exactive as it offered both high-quality MS1 and MS2 spectra. Due to flow injection, several MS^2 spectra (10 to 80) were acquired for every metabolite from which we chose 3 to 12 for the library. Using this flow injection/SIM/ddMS^2 method, we have generated almost 4000 MS^2 spectra for 444 metabolites after the first injection. 47 metabolites had to be re-injected at a higher concentration. LC library for 491 metabolites was generated in specific LC conditions.

New aspects

Using a novel flow injection/SIM/ddMS^2 method on a hybrid quadrupole oribtrap instrument, we developed a LC/MS library for > 490 metabolites.

A direct aqueous measurement of 25-hydroxyvitamin D in cellular environments by LC-MS/MS using the novel chemical derivatization reagent MDBP

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Einleitung

Chemical derivatization is often employed to enhance the ionization properties of vitamin D compounds. Cookson-type reagents such as 4-phenyl-1,2,4-triazoline-3,5-dione (PTAD) are well established, but require water-free experimental conditions. Traces of water inactivate the reagent and inhibit the derivatization reaction, thus making quantitative measurements in aqueous samples impossible without extensive drying steps. This drying step has the potential to change the distribution of metabolites within the sample, which is important for those samples, the structural integrity of the sample matrix cannot be compromised. We describe a novel liquid chromatography-tandem mass spectrometry (LC-MS/MS) assay for determining 25-hydroxyvitamin D3 (25(OH)D3) directly in aqueous cellular systems, using a new derivatization reagent, the ionic liquid 12-(maleimidyl)dodecyl-tri-n-butylphosphonium bromide (MDBP).

Experimenteller Teil

We synthesized the ionic liquid MDBP in a four-step reaction procedure and optimized the derivatization reaction conditions to achieve quantitative turnover. The derivatization strategy comprised a Diels-Alder reaction under physiological conditions in an aqueous environment, converting 25(OH)D3 into a permanently-charged quaternaryphosphonium ion. We compared MDBP with Amplifex to provide a comparison of the performance of the labels in aqueous solution. We measured the levels of 25(OH)D3 in four different human cell types, namely T cells, helper T cells, B cells and macrophages. The determination of 25(OH)D3 levels was directly performed in aqueous samples, thus maintaining the cellular integrity. We show the time-dependent uptake of 25(OH)D3 into the investigated cells, to demonstrate the applicability of the developed MDBP assay.

Ergebnisse und Diskussion

We observed very similar analytical figures of merit for MDBP as compared to the commercial Amplifex. The limit of detection (LOD) for 25(OH)D3 after derivatization with Amplifex was 0.05 ng/mL, in comparison to 0.10 ng/mL with MDBP. We demonstrated improved stability of MDBP in comparison to Amplifex, however, where MDBP was stable over weeks, in contrast to Amplifex's 2 hours. PTAD or Amplifex are limited to non- aqueous samples; these reagents do not to react in aqueous environments, because of the high reactivity of the activated N=N dienophile moiety. MDBP utilizes a less reactive, activated C=C bond, which enables the reaction in aqueous environments. As a result, the required derivatization time was longer for MDBP (quantitative turnover after 24 hours) as compared to Amplifex (<1 hour). MDBP onization efficiency for 25(OH)D3-MDBP increased approx.. 1000x in comparison to underivatized 25(OH)D3. The ESI response factors were 0.95 for MDBP and 0.98 for Amplifex, reflecting the permanently-charged phosphonium and quaternary ammonium groups of the derivatized molecules. The chemical derivatization of 25(OH)D3 with MDBP in cellular samples was performed under native physiological condition. without prior extraction and drying steps. All cellular systems were analyzed in activated and non-activated forms; measurement of the controls (without added 25(OH)D3) did not show significant signals for 25(OH)D3, thus excluding any endogenous sources for 25(OH)D3 in these samples. We performed an additional set of experiments that directly followed the uptake of supplemented 25(OH)D3 from the extra- to the intracellular region in cells to monitor the time-dependent distribution of 25(OH)D3 during incubation.

Neue Aspekte

Direct measurement of 25(OH)D3 in aqueous environment using the novel chemical derivatization reagent MDBP.

Imaging metabolites in wheat stem base - *Fusarium graminearum* interactions using high-resolution atmospheric pressure scanning microprobe MALDI mass spectrometry imaging (SMALDI-MSI)

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Introduction

Fusarium graminearum is a major pathogen of wheat (*Triticum aestivum*) causing the Fusarium head blight disease. Recently, its ability to colonize wheat via root infection has been reported. As the entry point to above-ground plant parts, the stem base is an important site of the wheat resistance against Fusarium root rot (FRR). The identification of metabolites related to pathogenesis and plant defense together with their localization, will significantly contribute to understanding this pathosystem. In this context, the atmospheric-pressure scanning microprobe matrix-assisted laser desorption ionization mass spectrometry imaging (AP-SMALDI MSI) system was used to localize metabolites related to *F. graminearum* invasion. Experiments were conducted in the FRR resistant wheat cultivar Florence-Aurore at different time points (10, 14 and 21 days after root infection).

Method

Several tissue sample preparation methods were optimized. Prior to sectioning, the stem base was embedded in 4% (w/v) carboxymethyl cellulose (CMC) using dry ice-hexane mixture. For cryosectioning, a cryomicrotome (HM 525 cryostat, Thermo Scientific, Dreieich, Germany) was used to obtain a 20 µm tissue thickness of both the infected and the uninfected section on a single glass slide. A solution of 150 µL, 2,5-dihydroxybenzoic acid (DHB) was applied by using a high-resolution matrix-preparation unit (SMALDIPrep, TransMIT GmbH, Giessen, Germany). Hereafter, a high-resolution atmospheric pressure scanning microprobe matrix-assisted laser desorption/ionization imaging source ("AP-SMALDI10", TransMIT GmbH, Giessen, Germany) with a Fourier transform orbital trapping mass spectrometer (Q Exactive, Thermo Scientific GmbH, Bremen, Germany) was used to rasterize the tissue section and to generate mass spectra.

Results

The “Mirion” software was used to generate high-quality *m/z* images (imaging bin width of ± 5 ppm). Metabolites were assigned based on high mass accuracy. By using the AP-SMALDI10 system, changes

in metabolic processes resulting from pathogen invasion could be detected and visualized. In the stem base of *F. graminearum* infected plants, we could visualize from 14 day on pathogenesis-related metabolites, such as the mycotoxins Enniatin A1 $[M+K]^+$ *m/z* 706.40394 and Enniatin B $[M+K]^+$ *m/z* 678.37264. These metabolites were not detected in the non-infected control samples. The observed infection path via the leaf sheath, which is wrapped around the stem, shows excellent correlation with previous microscopic observations. Visualizing structurally related metabolites simultaneously would be impractical with classical visualization techniques. In conclusion, using MS imaging has been found to be a suitable approach to gain novel insights into the topographical metabolite profiles during wheat-*Fusarium* interactions.

Novel aspects

Sample preparation for wheat stem base; understanding metabolite localizations in *Fusarium graminearum*-infected wheat stem base tissues sections

Key words

Fusarium graminearum, wheat stem base, plants, mass spectrometry imaging, metabolites

Automated electrochemistry/mass spectrometry for high-throughput analysis of xenobiotics

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Einleitung

Oxidation reactions play an important role during phase-I metabolism of xenobiotics in the human body. Phase-I reactions are catalysed mainly by cytochrome P450 enzymes. In the last 15 years, electrochemistry/electrospray ionisation mass spectrometry (EC/ESI-MS) has proven to successfully mimic many of these oxidation reactions in a purely instrumental approach. For many compounds that have been investigated by EC/ESI-MS, results obtained compete with established methods, e.g., microsome-based assays. Furthermore, EC/ESI-MS also allows the identification of unknown oxidation products as well as the elucidation of short-lived intermediates.

Experimenteller Teil

The electrochemical generation of oxidation products takes place in an electrochemical cell coupled online to high-resolution (HR)-ESI-MS. The results obtained at different potentials are shown in three-dimensional mass voltammograms. They plot the mass spectra versus the applied potential. With HR-ESI-MS, the oxidation products can be identified according to their accurate masses.

For drug development, it is necessary to analyse a large number of so-called pro-drugs, which is an expensive and time-consuming process. An automated system would significantly reduce analysis time. Until now, the automation of EC/ESI-MS has neither been described in literature nor been made commercially available. Combining an LC autosampler to the instrumental EC/ESI-MS setup and developing a powerful software tool enables high-throughput analysis with a purely instrumental approach.

Ergebnisse und Diskussion

In this study, EC/ESI-MS automation has been successfully applied to the investigation of phenothiazine, promazine, triflupromazine, thioridazine, chlorpromazine and fluphenazine. These analytes where chosen, because they show a comparable behaviour in the EC/MS coupling and in common in vitro methods. First, an optimization of different system parameters has been performed. The injection volumes as well as the flow rates were matched to determine the time periods during which the signals of the protonated species of the analytes were sufficiently constant. Furthermore, rinsing steps were introduced in order to clean the system and to prevent carry-over effects. In the following, the necessary time interval between the application of two potential ramps was determined. Thus, the oxidation products are washed out of the electrochemical cell. This allowed to perform several EC/MS measurements with a single injection performed by the LC autosampler. The results from the manual and the automated approach were

compared and the reproducibility was determined. Within this work, it has been shown that the automated EC/MS coupling is a powerful alternative to established EC/MS approaches. The automated system is less time consuming and may thus allow to carry out significantly more analyses in a given period of time at lower costs.

Neue Aspekte

Development of an automated high-throughput system for EC/HR-ESI-MS using an LC autosampler

Stichworte

HR-ESI-MS, Electrochemistry, Metabolism, Automation

Probing plant Maillard reaction by mass spectrometry in model peptide systems

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Introduction (120)

Glycation is a post-translational modification formed in the reaction of protein lysyl and arginyl residues with reducing sugars or dicarbonyl products of their degradation. This process leads to formation of advanced glycation end products (AGEs), accumulating during thermal processing of foods and demonstrating clear pro-inflammatory effects after consumption and intestinal absorption in human gut. Surprisingly, high contents of AGEs were found in unprocessed plant tissues [1], and the pathways of their formation differed essentially from those described for mammals [2]. Obviously, different physiological conditions and rich sugar patterns are the reasons for this. Therefore, here we address *in vitro* and *in vivo* reactivities and glycation potentials of individual plant sugars by a variety of mass spectrometric methods.

Methods

Peptides Ac-AFGSAKASGA-NH_2 and Ac-AFGSARASGA-NH_2 were synthesized by solid phase peptide synthesis using an Fmoc strategy, and glycated *in vitro* during 42 days at 22°C with equimolar amounts of twenty individual plant sugars in 0.1 mol/L sodium phosphate buffer (pH 7.4, 50 µL) containing 18 µmol/l $FeSO_4$. The peptide- and carbohydrate-related products were analyzed by UHPLC-ESI-QqTOF-MS and GC-EI-Q-MS, respectively. Structural characterization of the products relied on characteristic fragmentation patterns. The plant material was obtained from *Arabidopsis thaliana* and *Brassica napus* plants, grown for 42 days according to Bilova et al [2]. Proteomic analysis relied on tryptic digestion of protein extracts and nanoRP-UHPLC-LIT-Orbitrap-MS data-dependent acquisition (DDA). The patterns of carbohydrates and dicarbonyls were evaluated with GC-EI-Q-MS.

Results and discussion

Among the carbohydrates tested, glucose-6-phosphate demonstrated the highest reactivity – depending on the sequence, approximately 85 - 100% of initial peptide amount was degraded after 42 days. In contrast, glucose and sucrose were completely non-reactive. In total, 46 and 105 products were detected in the incubations with lysine-and arginine-containing peptides, respectively. Thereby, glucose-6-phosphate, fructose-6-phosphate, ribulose, and ribulose-1,5-diphosphate resulted in the richest product patterns in the model reactions with the lysine-containing peptide, whereas glyceraldehyde-3-phosphate, dihydroxyacetone phosphate, ribulose, and ribulose-1,5-diphosphate produced the highest diversity of products with arginine-containing sequence. Thus, the key players of the principle primary metabolism pathways (glycolysis and Calvin cycle) turned to be the most potent glycation agents. Remarkably, these sugars yielded specific patterns of glycation and/or oxidation product that corresponded well to prospective AGE-specific formation mechanisms and could be confirmed by metabolomic data. Considering *in vivo* plant carbohydrate patterns in the context of characteristic sugar reactivities and glycation potentials revealed relatively high abundance of potent glycation agent that might explain unexpectedly highly abundant patterns of AGEs in plants [2].

Significance (20)

The principle metabolites of glycolysis and Calvin cycle are the most potent glycation agents in plants

[1] Bechtold,U.; Rabbani,N.; Mullineaux,P.M.; Thornalley,P.J. Quantitative measurement of specific biomarkers for protein oxidation, nitration and glycation in Arabidopsis leaves. 2009. Plant J. 59 (4), 661-671

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Intensity Independent Filtering of FT MS and FT MS/MS Spectra for Shotgun Lipidomics

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Shotgun lipidomics provides a quantitative snapshot of total lipid extracts composition and typically relies on the interpretation of high resolution MS and MS/MS spectra. These spectra could comprise > 100.000 signals, however only a few of those represent bona fide molecular ions of lipids. Depending on the lipid class and analysis conditions the signal intensities vary > 1000-fold and they could not be distinguished from noise by some arbitrary cut-off threshold. Here we report on a signal intensity independent method to eliminate noise from shotgun spectra, which dramatically simplifies and accelerates processing of complex FT MS and FT MS/MS datasets with uncompromised lipidome coverage and quantification accuracy.

Experimenteller Teil

Bovine heart PC extracts and lipid standard mixtures were analyzed by shotgun lipidomics on a QExactive instrument. FT MS and FT MS/MS were acquired at target resolution of 140.000 (at m/z 200) and AGC were set to 2E6 and 2E4, respectively. Each FT MS/MS was 11 times acquired and separately processed by a in house developed software. Lipids were identified and quantified by LipidXplorer software [1].

Ergebnisse und Diskussion

We investigated the signal properties of PC and PC *O*- adduct ions in FT MS/MS- spectra whose abundance differed by 200-fold. The abundance of noise signals varied within the spectra in m/z-dependent manner and differed by > 100-fold concomitantly with the abundance of corresponding precursors. Therefore, arbitrary thresholds of signal-to-noise and/or peak intensity uniformly applied to all spectra in a dataset could bias the interpretation. At the same time, irrespectively of their intensity, > 90% of noise signals were only detected in individual scans with low repetition rates, while signals related to bona fide PC/PC O- fragments were detected with high (> 75%) repetition rate. We therefore tested if repetition rate could be used as intensity independent threshold to eliminate noise.

For repetition rate filtering, the m/z range of each FT spectra was segmented into 1 mDa bins and signals were sorted by their accurate m/z. Signals having the repetition rate < 65% within a search window +/- 3 mDa were eliminated. We found that this procedure reduced the dataset size by > 95%, while still being able to recognize 103 molecular species of PC/PC O- having the signal-to-noise ratio above the value of 10. When the same dataset was reduced to a similar size by applying a signal intensity cut-off threshold, 47% of these species were lost. In summary, repetition rate filtering enabled efficient reduction of shotgun datasets without compromising the confidence of identification and quantification of lipids, hence eliminating a major bottleneck in high throughput shotgun lipidomics.

Neue Aspekte

Intensity independent filtering eliminated > 95% noise without compromising the performance of shotgun lipidomics

Referenzen

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Mass spectrometry evaluation of the Etanercept physicochemical properties

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Etanercept is a fusion protein combining the Fc domain of human IgG1 to the extracellular portion of the TNF receptor-2, is an effective drug for different types of arthritis treatment. Etanercept went off-patent in 2015 in Europe and the pharmaceutical companies have started producing the biosimilar versions of this protein [1]. Confirmation of the biosimilarity is dependent to proving the comparability between the biosimilar product and the originator brand. Mass spectrometry is the cornerstone of the different analytical techniques which are used for investigating the composition and structural characteristics of these therapeutics [2]. In this work, the results from the evaluation of the Etanercept structure based on mass spectrometric analysis at different levels (top-down, middle-down and bottom-up) will be reported.

Experimenteller Teil

Isoelectric focusing was performed using Bio-Rad's Criterion™ apparatus and the Criterion™ IEF Gel with the pH of 3–10 was used for running the proteins. Running condition was based on the manufacturer recommendations.

Desialylated and deglycosylated Etanercept were prepared by adding the Promega deglycosylation mix and the neuraminidase based on the manufacturer recommendations.

Papain digestion was carried out by using the 1:100 W/W enzyme to protein ratio in a reaction buffer and incubation at 37°C for 4 h.

Identity was verified through tryptic peptide mapping analyzed by RP-UPLC coupled to Orbitrap Q Exactive™ mass spectrometer.

The Top-down and the middle-down analysis were performed by direct injection of desalted molecules into a Q-TOF mass spectrometer.

Ergebnisse und Diskussion

According to common guidelines, the primary sequence of the reference and the biosimilar version of a therapeutic protein must be the same. Therefore, in the first step, the in-solution digestion method was used for confirmation of the primary structure of the Etanercept. This method provided the verification of the sequence coverage with respect to the theoretical sequence being 36%. Although the primary structure of the Etanercept was verified, the level of the coverage is not satisfactory. Considering the high degree of glycosylation, the next steps for increasing the sequence coverage would be using different proteases for protein digestion and the deglycosylated Etanercept as the starting material for peptide mapping procedure.

Etanercept is a highly glycosylated fusion protein which contains several N- and O-glycosylation [3]. This amount of glycosylation results in a high heterogeneity of the drug product. As a result, Etanercept drug product is highly heterogeneous consisting of many

similar species. The charge heterogeneity of the species of Etanercept was investigated through IEF analysis. The Etanercept pI of the target species mostly lie in the range of 4.8 to 5.8 and these species are the results of different PTMs especially glycosylation [4]. Thus, direct injection of the Etanercept into the QTOF mass spectrometer evidenced a high degree of the heterogeneity which resulted in a mass spectrum which could not be deconvoluted. Consequently, the heterogeneity was tried to be decreased by cutting the sugars and digesting the Etanercept to the Fc and TNFr fragments [5]. Even after using deglycosylated Etanercept, the exact mass of the Etanercept was not resolved. The best result was gained from the injection of Etanercept digested with papain. These data suggest that fractionation and generating less heterogeneous molecules for getting the high quality and precise data are essentially needed.

Neue Aspekte

Defining a frame for mass spectrometric analysis of therapeutic proteins

Referenzen

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Age-related glycation hotspots in plant proteome

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Introduction

Glycation is usually referred to as a non-enzymatic reaction of protein amino and guanidino groups with reducing sugars and α-dicarbonyls. Resulting advanced glycation end products (AGEs) accumulate in mammalian tissues continuously throughout their life span, and are known as the markers of inflammation-related diseases and ageing. Surprisingly, despite of high tissue sugar contents and high rates of oxidative processes, age-related formation of AGEs in plants was not addressed so far. Recently, we characterized constitutive glycation patterns in *Arabidopsis thaliana* and *Brassica napus*, and discussed potential precursors and mechanisms of AGE formation in plants [1]. Here we consider this problem in a time dimension, and address possible mechanisms of observed site-specificity in age-dependent advanced glycation of plant proteins.

Experimental section

Arabidopsis plants (6-12-week old) were characterized by a pattern of stress markers, as well as metabolome (GC-EI-Q-MS) and proteome (nanoLC-ESI-Orbitrap-LIT-MS/MS-DDA) profiling. Identification of glycation sites and protein annotation relied on Sequest search against an *A. thaliana* database and manual confirmation of sequence assignment. Thereby, characteristic *m/z* increments and side chain fragmentation patterns were considered. Label-free quantification of individual glycation sites relied on integration of the corresponding peptide signals in extracted ion chromatograms at characteristic t_R using LCQUAN™ software. The protein functions were annotated with MapMan tool (http://mapman.gabipd.org). Sequence consensus moieties (25 residues prior and after AGE-modified sites) were assigned by Weblogo (http://weblogo.berkeley.edu/), whereas protein homology modeling relied on YASARA software [2].

Results and discussion

In general, plant protein glycation patterns were relatively stable in time, and only a limited number of proteins demonstrated an age-related increase of AGE levels. The most of the corresponding glycation sites contained arginine residues and represented the proteins involved in transcriptional regulation and protein metabolism. The AGE patterns dominated by N^{ϵ}-(carboxymethyl)lysine (CML) and hydroimidazolones (Glarg and MG-H), originating from α-dicarbonyls - glyoxal and methylglyoxal. These patterns can be explained by an age-related enhancement of carbohydrate oxidation. Surprisingly, despite of its non-enzymatic nature, AGEs were formed at specific sites in protein sequence. Such a site-specific increase of glycation levels was confirmed by label-free protein quantification – 1.5-28 fold. The existence of a conservative protein patterns, susceptible to age-related glycation, clearly indicates the existence of "glycation hotspots" in plant proteome. This phenomenon was already shown for some animal proteins and, most probably, might be underlined by specific protein sequence or/and structure motifs [3]. Indeed, comparison of glycation-specific sequence motifs in plant proteome with those earlier described in mammalian proteins revealed similar patterns of highly represented ionic (K,R,E,D) and non-ionic residues (L,V,A,P) in close proximity to the glycation sites. Moreover, characteristic structural motifs, containing anionic residues (E,D) were found in close proximity (typically less than 5.0 Å) to the majority of "glycation hotspots". We assume, that these residues take part in a not yet known catalytic mechanism of the lysine or arginine glycation or/and they can stabilize the basic hydroimidazolones (MG-H and Glarg), and increase the times required for their degradation and further conversion into other AGEs, that is in good agreement with our previous *in vitro* data [4]. Obviously, for the complete

structural and functional characterization of the “glycation hotspot” patterns, in-depth analysis of plant glycated proteome is required.
The research was supported by the Russian Scientific Foundation (project no.16-16-00026).

Novel aspects
A pattern of plant proteins demonstrates an age-dependent increase of glycation level.

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3. Barnaby, O. S., Cerny, R. L., Clarke, W., and Hage, D. S. (2011). *Clin. Chim. Acta* 412, 277-285

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Key words: α-dicarbonyls, AGEs, aging, Arabidopsis thaliana, mass spectrometry, oxidative stress, protein glycation, proteomics

Analysis of UV-induced DNA–protein cross-links in a chromatin model

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Nucleic acid-protein interactions are pivotal to numerous cellular processes including structural and catalytic activities of RNA- and DNA-containing protein complexes. The identification of these transient interaction sites is crucial for our understanding of nucleic acid-mediated processes. We recently described a search algorithm that allows analysis of UV-induced peptide–RNA cross-links down to the level of single amino acids [1]. We have now focused on chromatin, the most prominent cellular DNA-protein complex, comprised of the genomic DNA that is wrapped around four core histone proteins forming repeating units of nucleosomes that in turn are bound by linker histones. By combining UV-induced cross-linking and mass spectrometry we are able to deduce individual protein-DNA cross-link sites and map them to the nucleosome structure [2].

Experimenteller Teil

We used individual linker histones as well as oligonucleosomal arrays to elucidate protein-DNA cross-links after UV irradiation. Human linker histone H1.4 and chicken linker histone H5 were mixed with a 187 bp DNA fragment whereas oligonucleosomal arrays were reconstituted *in vitro* using recombinant core and linker histones and DNA containing 12 nucleosome positioning sequences. Linker histone-DNA complexes or chromatin arrays were irradiated with UV light (254 nm). Following enzymatic hydrolysis of DNA and proteins, non-cross-linked DNA was removed by C18 reversed phase and the samples were enriched for peptide-DNA cross-links with TiO_2 affinitiy chromatography. Cross-links were analyzed on a hybrid quadrupole-orbitrap mass spectrometer (Q Exactive HF, Thermo Scientific). Data analysis was performed using the RNP^{xl} pipeline of OpenMS as described previously [1].

Ergebnisse und Diskussion

In contrast to RNA, where cross-links are mainly observed to uracil, we have identified thymine and cytosine nucleobases as well as the sugar-phosphate moiety of DNA to cross-link to proteins. Given the lysine- and arginine-rich nature of histone proteins, we mainly detected cross-links of nucleobases to lysine residues but also to leucine, tyrosine and proline residues. Interestingly, cross-links to the sugar-phosphate moiety only occurred on histidine residues. We confirmed these novel types of cross-links by performing experiments with $^{15}N/^{13}C$-labeled DNA.

Altogether, we observed cross-links to linker histones (in the context of single histones) and to all four core histone proteins as well as linker histones within oligonucleosomal arrays. The cross-linking sites mapped to the globular domains of H5 and H1.4 and the N-terminal and C-terminal domains, which have not been structurally annotated to date. Moreover, the relative positions of cross-linked histone residues and DNA in the available structures of the nucleosome [2] and the nucleosomal core particle [3] are consistent with our findings. Hereby, the observed proximity of DNA and cross-linked amino acids demonstrate the specificity of our experimental approach. All in all, this proves that UV-induced protein–

DNA cross-linking analysis provides a versatile tool to characterize protein–DNA complexes in general and will contribute to our understanding of chromatin structures.

Neue Aspekte

Mass spectrometric analysis of UV-irradiated DNA-protein complexes reveals cross-links to nucleobases and the sugar-phosphate backbone of DNA.

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[3] Luger K, Mäder AW, Richmond RK, Sargent DF, Richmond TJ. (1997). Crystal structure of the nucleosome core particle at 2.8 A resolution. Nature 389(6648):251-60

Sarah Stow
Jody May
John McLean

Standardised Collision Cross Section Measurements by Single Static Drift Field Ion Mobility Instrument in an Interlaboratory Study

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Outline

1) Resolving Instrumental Contributions

Instrument design overview

How well can we know pressure, temperature, length and voltage?

2) Standardising the Measurand (Collisional Cross Section, ^{DT}CCS)

Terminology: *precision*, *repeatability*, *reproducibility*, *bias*, *accuracy*, *uncertainty*

Agilent Reference System

Assessment of measurement uncertainty (EURACHEM)

International inter-laboratory study (*reproducibility*)

3) Study Results and Ongoing Work

Metabolites, lipids, peptides, proteins

Publication plan

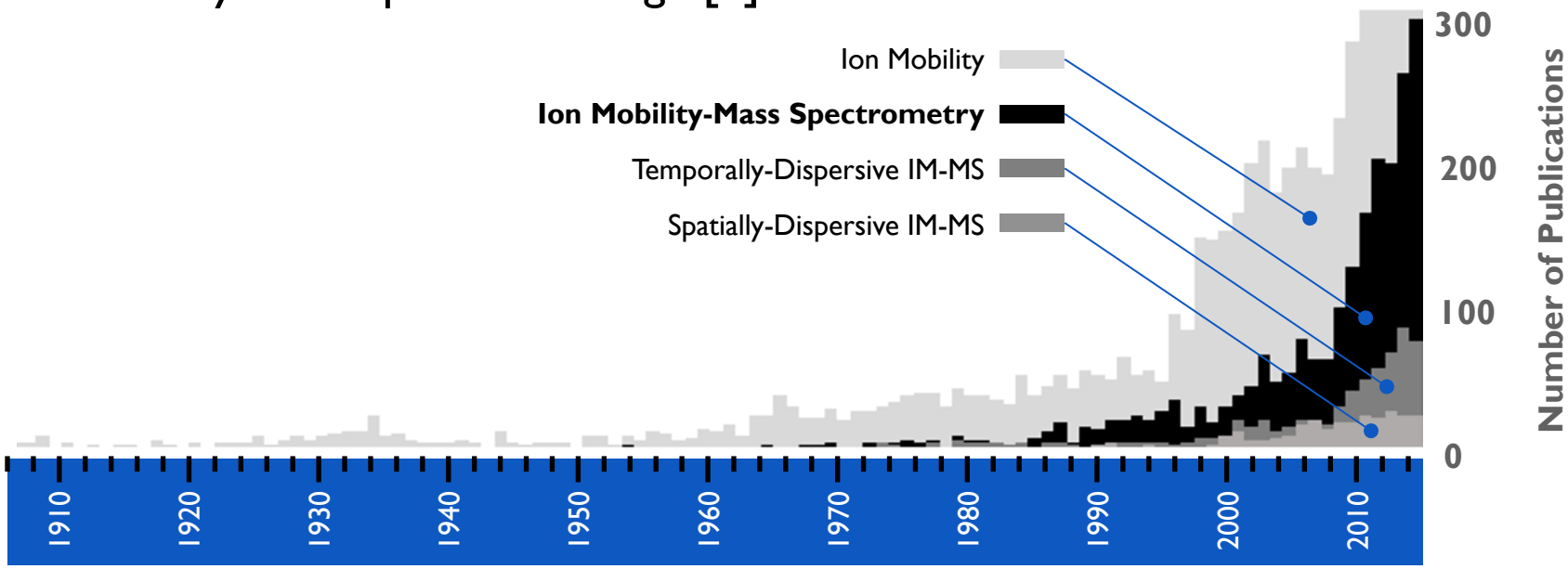
Improving low molecular mass measurements

Ion Mobility – Mass Spectrometry

Broader Interests – Driving Standardisation and Method Development

- Substantial increase in literature interest for Ion Mobility-Mass Spectrometry (IM-MS) [1].

- Adding IM between LC and MS is a powerful way to increase method selectivity and improve coverage [2].



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Separation Technologies and Identification Applicability

Can Ion Mobility be used to Aid Compound Annotation and Identification?

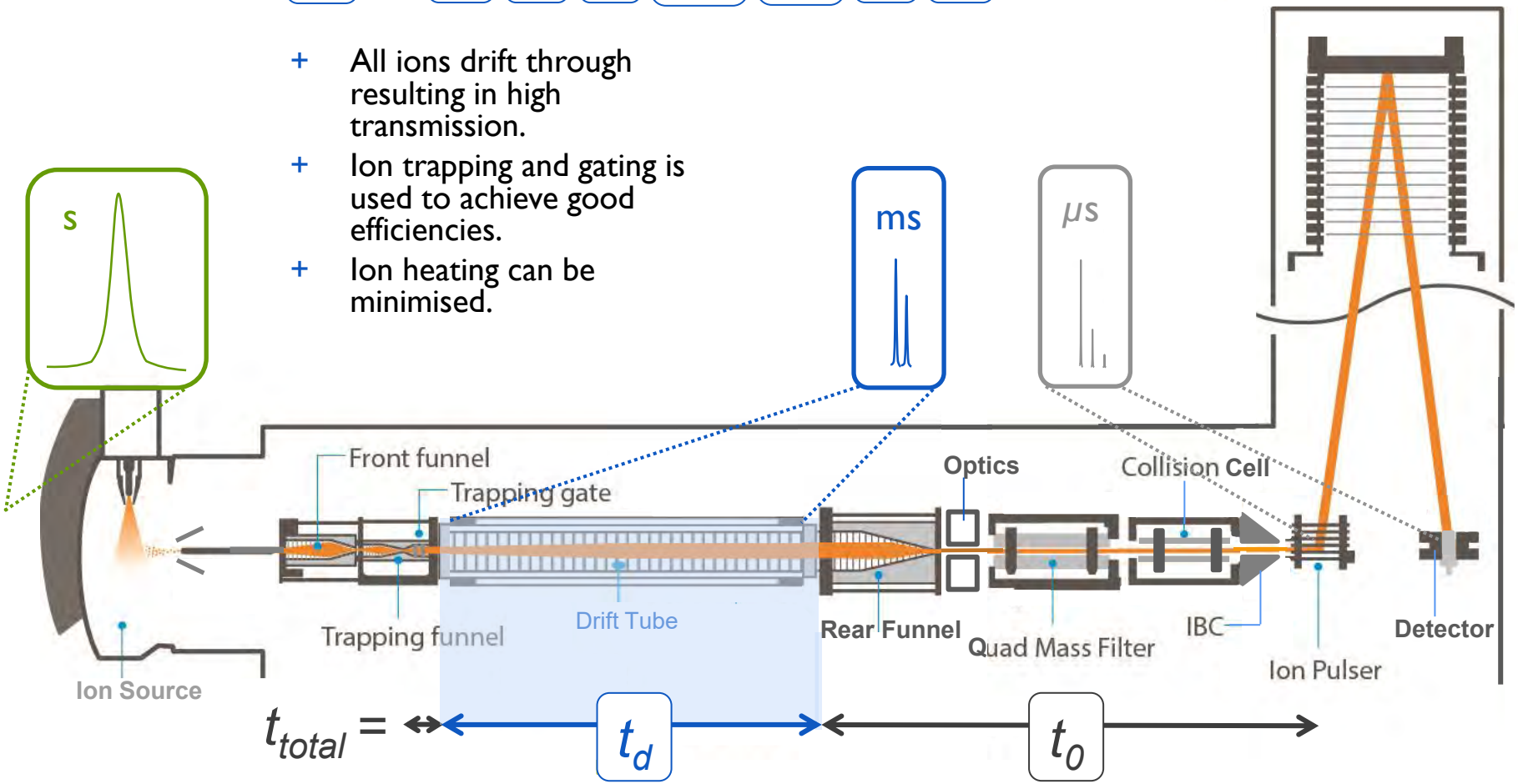
	Gas Phase (GC)	Liquid Phase (LC)	Ion Mobility (IM)	Mass Spectrometry (TOF-MS)
Analytical Measure	Ret. Time	Ret. Time	Flight Time	Flight Time
Property Measured	Partition Coeff.	Partition Coeff.	CCS or Ω	*m/z*
	Resultant from the analyte, stationary and mobile phases and temperature influences		A property of the analyte, drift gas and temperature	A property of the analyte
System Precision	1% Rel. RT	Variable	Typ. 2%	< 1 ppm
Database Compatible	Indices - Yes	Limited	Possible?	Yes

Instrumental Design of Low-Field Drift Cell System

Addition of Drift Tube IM to QTOFMS System

$t_d \not\propto T \; P \; L \; m_b \; m_i \; z \; E$

- + All ions drift through resulting in high transmission.
- + Ion trapping and gating is used to achieve good efficiencies.
- + Ion heating can be minimised.



Determining Drift Time (t_d) and ^{DT}CCS

Stepped-field Methodology

Stepped-field:

Classical determination of ^{DT}CCS values requires changing the drift-field and recording of apparent drift times.

Plot of 1/ΔV against observed drift time is linear (low-field behaviour).

Intercept used to correct to the true drift time (**t_d**).

Single-field:

Transient peaks allow only enough time for one field strength to be used.

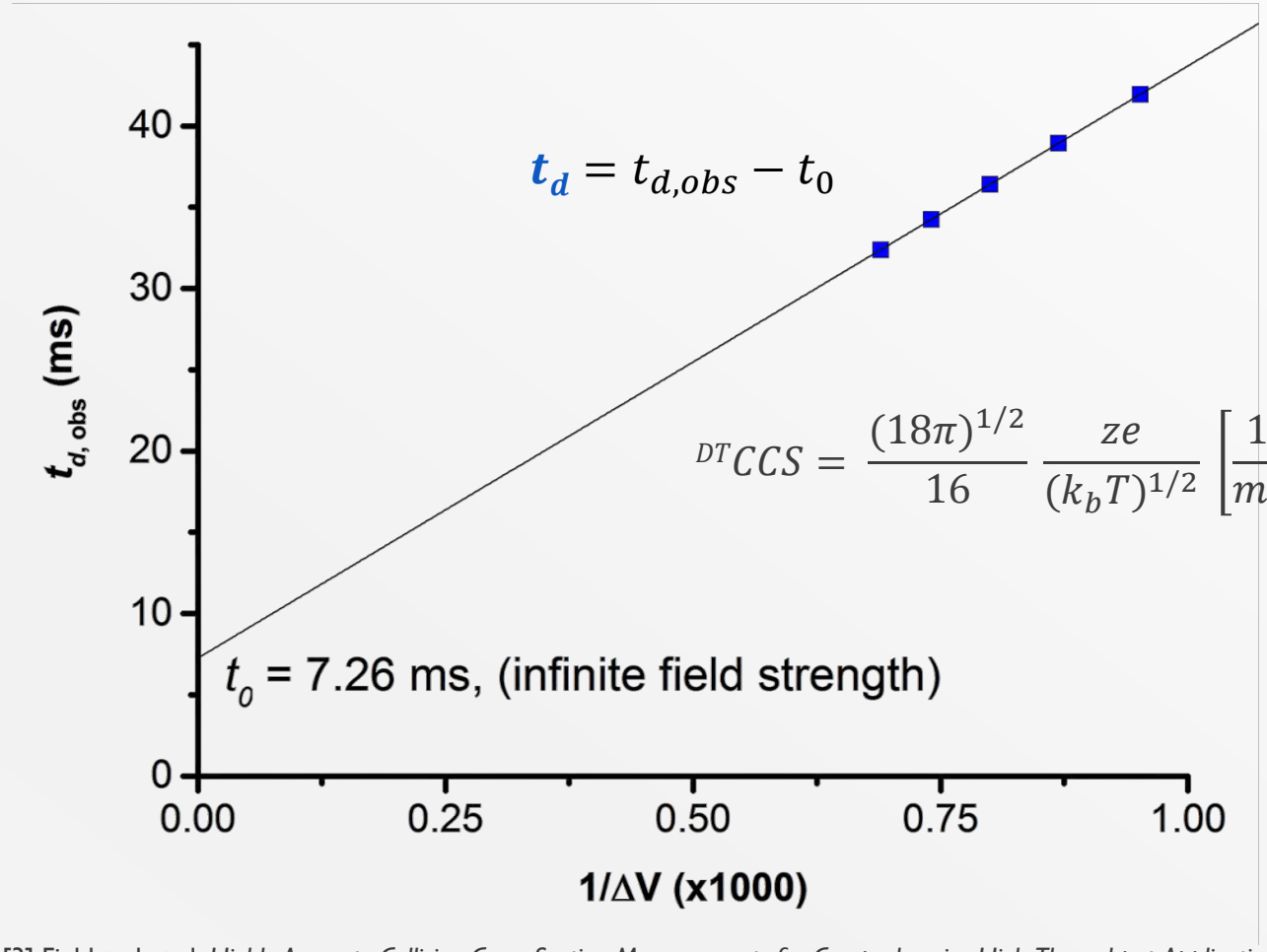
Use drift times of calibrant ions ("known" ^{DT}CCS values) to perform *universal linear calibration*.

Calibration function applied to IM-MS or LC × IM-MS files.

[3] Fjeldsted et al, *Highly Accurate Collision Cross Section Measurements for Comprehensive High Throughput Applications*, 2016, 64th ASMS, San Antonio, USA.

Determining Drift Time (t_d) and ^{DT}CCS

Stepped-field Methodology



$$^{DT}CCS = \frac{(18\pi)^{1/2}}{16}\frac{ze}{(k_bT)^{1/2}}\left[\frac{1}{m_I}+\frac{1}{m_B}\right]^{1/2}\frac{t_dE}{L}\frac{760}{P}\frac{T}{273.15}\frac{1}{N}$$

[3] Fjeldsted et al, *Highly Accurate Collision Cross Section Measurements for Comprehensive High Throughput Applications,* 2016, 64th ASMS, San Antonio, USA.

Inter-Lab Study

Determining the Limits of ^{DT}CCS Measurement Uncertainty

- Use Monte-Carlo simulation to predict the uncertainty of ^{DT}CCS measurement.
- Establish reference values for calibration ions (="known" values).
- Execute a study at several sites internationally to assess experimental reproducibility.
- Test a universal calibrated *Single Field* method that adheres to fundamental zero field equation (Mason-Schamp).
- Publish results.

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Terminology

Speaking the Same Language [1,2]

- **Precision**: (measurement precision) is a measure of how close results are to one another…it is calculated from results obtained by carrying out replicate measurements on a suitable material under specified conditions.
  - *Repeatability*: measure of the variability in results when a measurement is performed by a single analyst using the same equipment over a short timescale.*
  - *Reproducibility*: measure of the variability in results between instruments/laboratories.*
- **Bias** (or **Trueness**): comparison of the mean of the results ($\bar{x}$) from the candidate method with a suitable reference value ($\bar{x}_{ref}$). Can be given in absolute or relative terms.
- **Accuracy**: expresses the closeness of a single result to a reference value. Accuracy is, therefore, normally studied as two components: '*trueness*' and '*precision*'.
- **Uncertainty**: an interval associated with a measurement result which expresses the range of values that can reasonably be attributed to the quantity being measured. An uncertainty estimate should take account of all recognised effects operating on the result.

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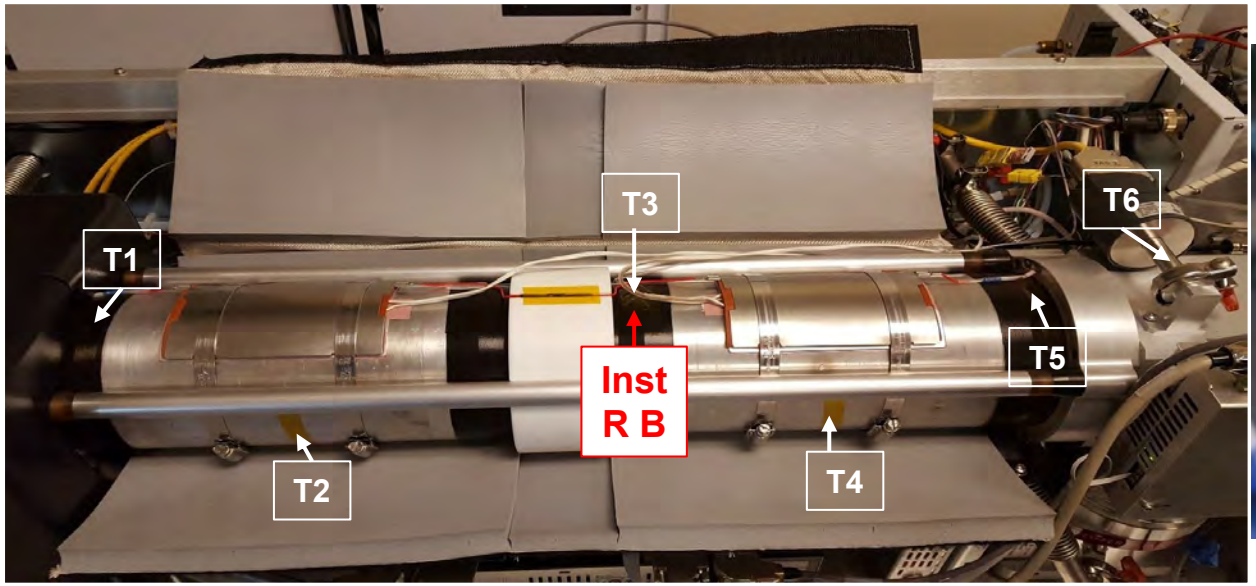
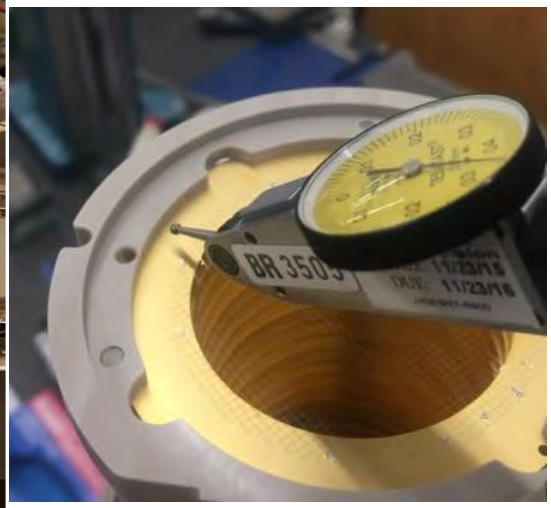
Agilent Reference System (Santa Clara, USA)

Providing Best Estimates for True ^{DT}CCS Values

- Additional grids added to afford better $t_{d,obs}$ measurements.
- Axial temperature profile across drift cell measured.
- Independent high precision voltage measurements made.
- Drift cell length physically measured with respect to grids.
- => Measurement uncertainty contributions of *L*, *T*, and *V* well-understood.





Assessing Instrumental Contributions to Uncertainty

Investigations at BOKU

- Construct an uncertainty estimate for drift time, t_d using EURACHEM guidelines
- Restate the zero field (Mason-Schamp) equation to model impact of key input quantities
- Propagate error and calculate total expanded uncertainty using Monte Carlo simulation

$$t_d = \frac{\Omega}{10^{20}} \frac{16}{(18\pi)^{1/2}} \frac{1}{ze(k_b)^{1/2}} \left[\frac{1}{\sqrt{\frac{m_I + m_B}{m_I m_B}}}\right] \frac{L^2}{V_{entr} - V_{exit}} \frac{P}{760} \frac{101325}{T^{1/2}}$$

Parameter	Unit	Value	Uncertainty	min	max	Distribution
L	m	0.78302	+/- 0.000088	0.782932	0.783108	normal
T	K	299.4	+/- 0.5	298.9	299.9	normal
P	Torr	3.945	+/- 0.0079	3.937	3.953	normal
V_{entr}	V	1474	+/- 2	1472	1476	uniform
V_{exit}	V	224.0	+/- 2.5	221.5	226.5	uniform

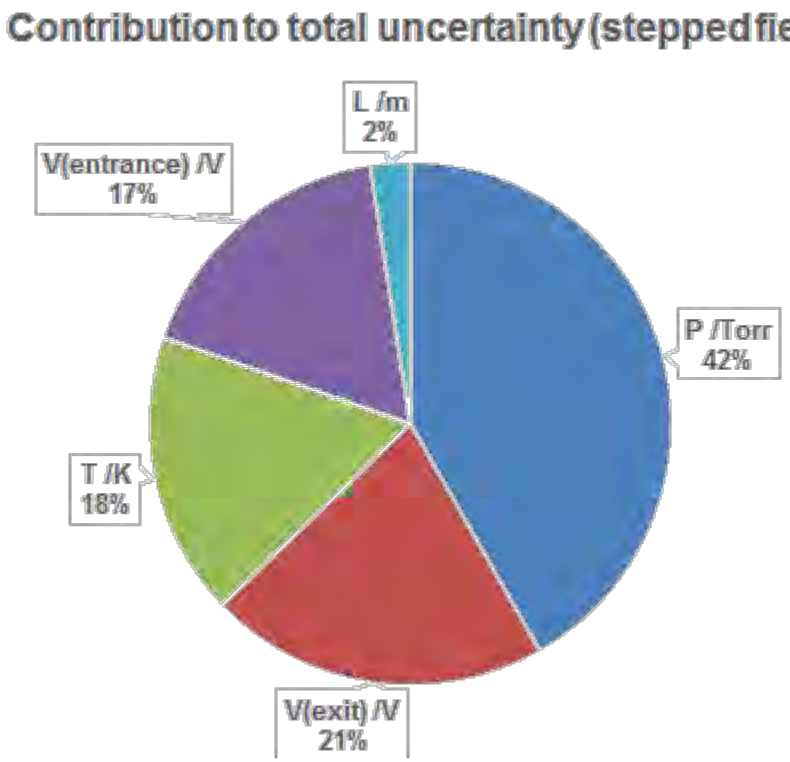
EURACHEM - Quantifying Uncertainty in Analytical Measurement, 3rd Edition (2012)

Assessing Instrumental Contributions to Uncertainty

Uncertainty Simulation for Agilent Reference System

Uncertainty for drift time calculated for Tune Mix ion *m/z* 322 (100,000 iterations)

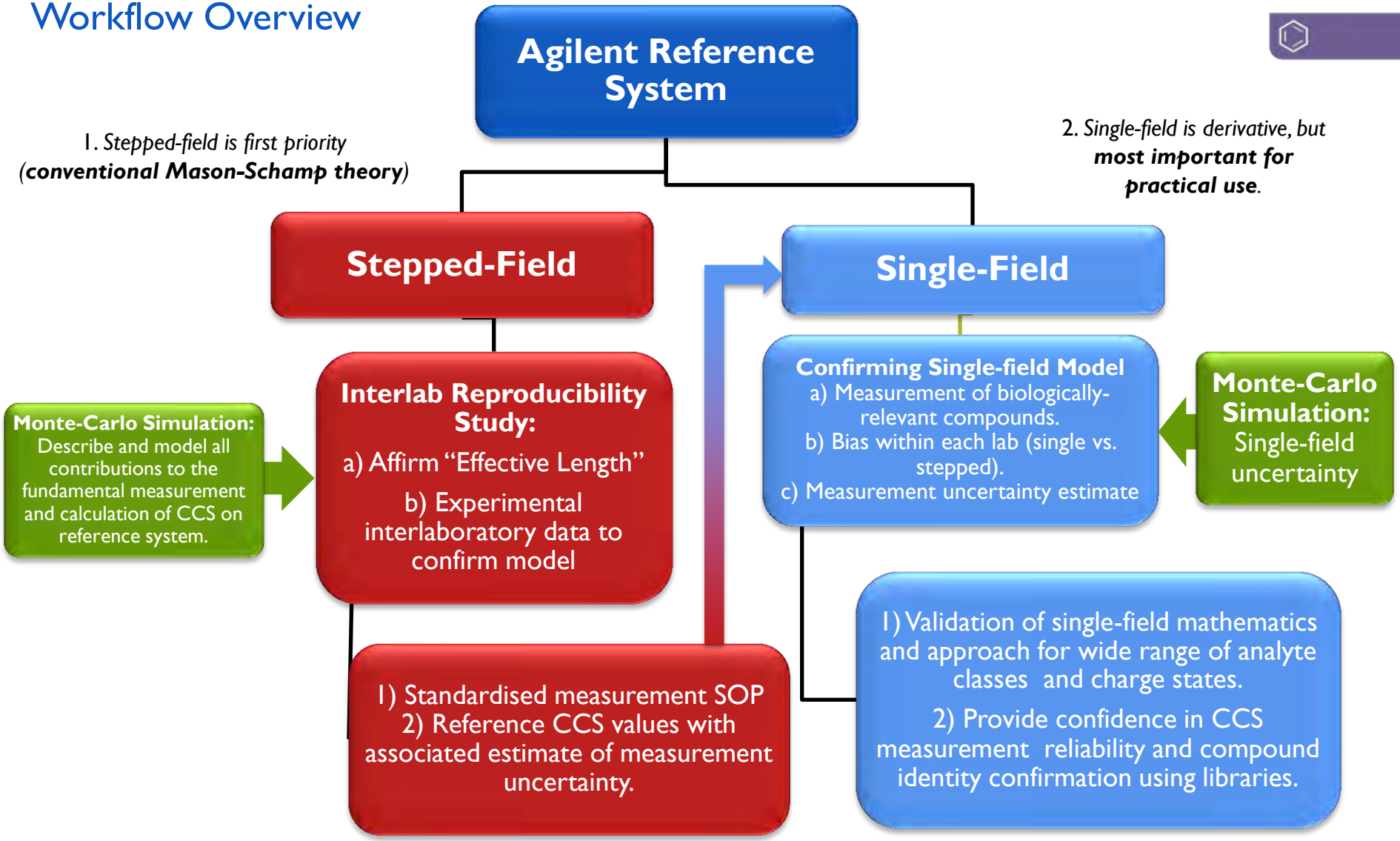
$t_{d,\,obs}$ (ms)	Standard deviation (ms)	Relative standard deviation - %
16.76	0.05	0.26



- Distributed contributions – with pressure and voltages being the most significant.
- The total expanded uncertainty is estimated to be 0.52% (coverage factor 2, corresponding to approximately 95% CI).

Standardisation Strategies: Stepped- and Single-Field

Workflow Overview



Agilent Reference System Results: Measured Values

Stepped-field Measurements of Agilent Tune Mix Ions as ^{DT}CCS Standards

Positive Ion Mode

Tune Mix Ion	$^{DT}CCS_{N_2}$ (Å^2)	%RSD
118	121.30 ± 0.20	**0.17%**
322	153.73 ± 0.23	**0.15%**
622	202.96 ± 0.27	**0.14%**
922	243.64 ± 0.30	**0.12%**
1221	282.20 ± 0.47	**0.17%**
1521	316.96 ± 0.60	**0.19%**
1821	351.25 ± 0.62	**0.18%**
2121	383.03 ± 0.64	**0.17%**
2421	412.96 ± 0.58	**0.14%**
2721	441.21 ± 0.59	**0.13%**

Negative Ion Mode

Tune Mix Ion	$^{DT}CCS_{N_2}$ (Å^2)	%RSD
112	108.23 ± 0.20	**0.19%**
301	140.04 ± 0.29	**0.21%**
601	180.77 ± 0.21	**0.12%**
1033	255.34 ± 0.32	**0.13%**
1333	284.76 ± 0.31	**0.11%**
1633	319.03 ± 0.70	**0.22%**
1933	352.55 ± 0.27	**0.08%**
2233	380.74 ± 0.31	**0.08%**
2533	412.99 ± 0.31	**0.07%**
2833	432.62 ± 0.35	**0.08%**

These data include measurements acquired under the 4 tune setting options over 3 separate days.

Inter-Lab Study Results: Measured Values

Stepped-field Approach: Normalised to Agilent Reference System

- Update applied to Agilent Reference System data to consider high-precision voltage, and temperature readings.

- For 3-lab study, the total corrections on raw data are additive and applied as an "*effective length*" (L_{eff}) for stepped-field calculations of tune ions.

1. $\sqrt{\frac{CCS_{BOKU(78.12)}}{CCS_{Agilent)}}} = \frac{121.97}{121.30}$

2. $\sqrt{CCS\ ratio} * 78.12 = L_{eff}$

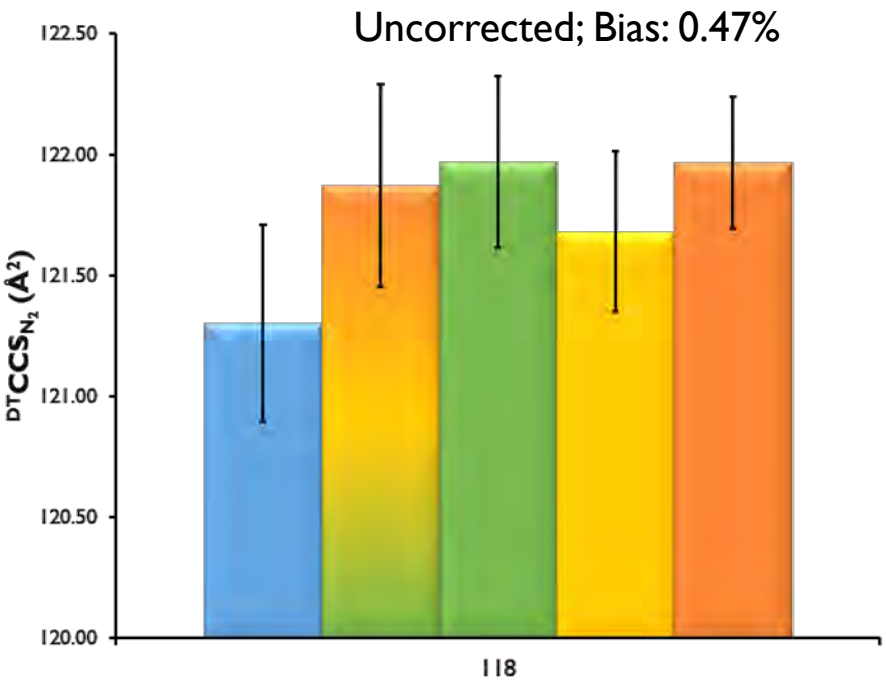
3. $\overline{L_{eff}}\ across\ all\ tune\ ions, 3\ labs, 4\ tune\ modes, 3\ days$

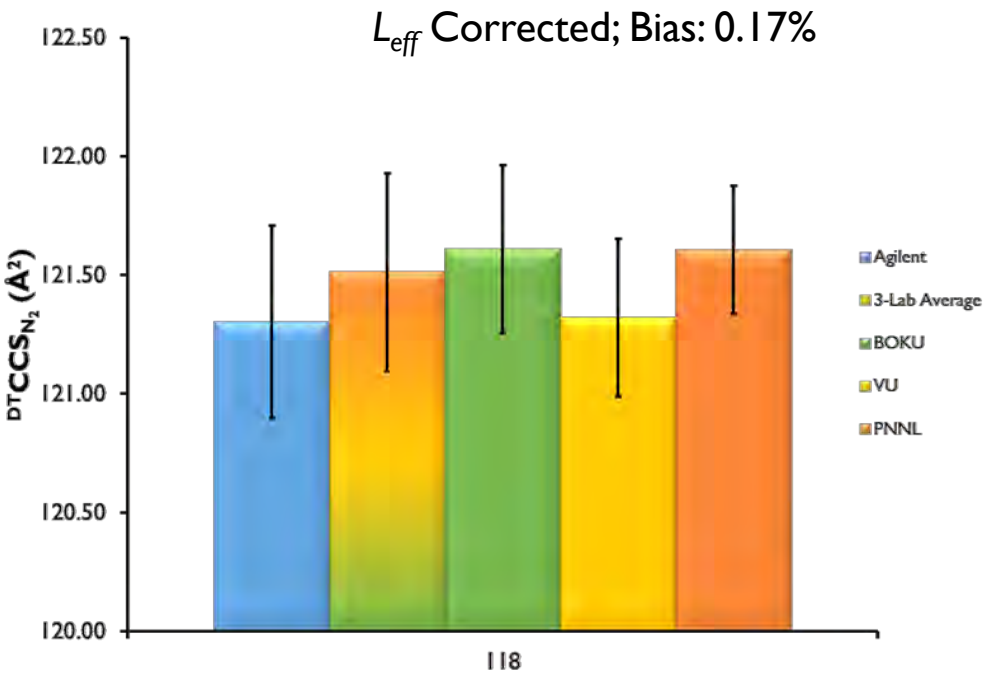
Inter-Lab Study Results: Measured Values

Stepped-field Approach: Normalised to Agilent Reference System

- Update applied to Agilent Reference System data to consider high-precision voltage, and temperature readings.

- For 3-lab study, the total corrections on raw data are additive and applied as an "*effective length*" (L_{eff}) for stepped-field calculations of tune ions.

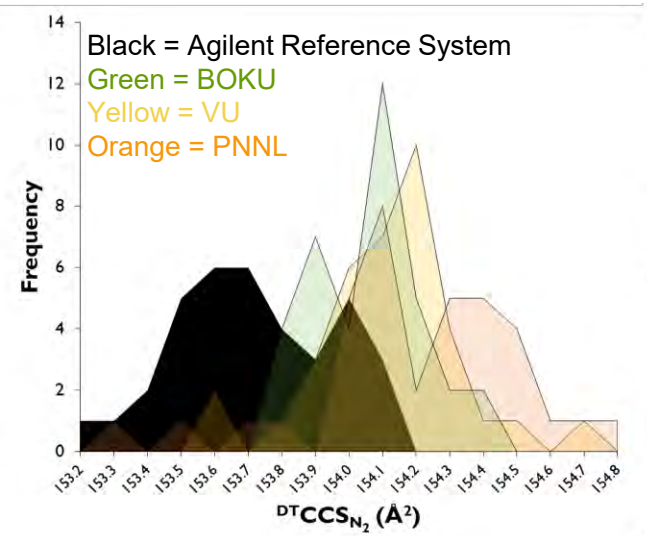




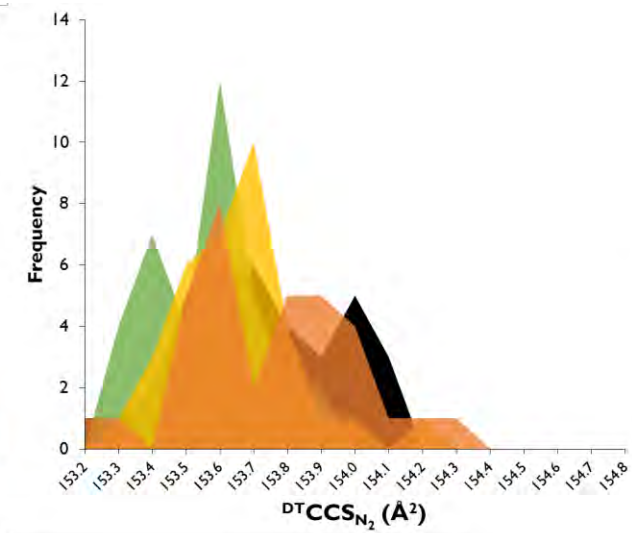
Interlab Study Results: Agreement on L_{eff}

How Different are the Instruments?

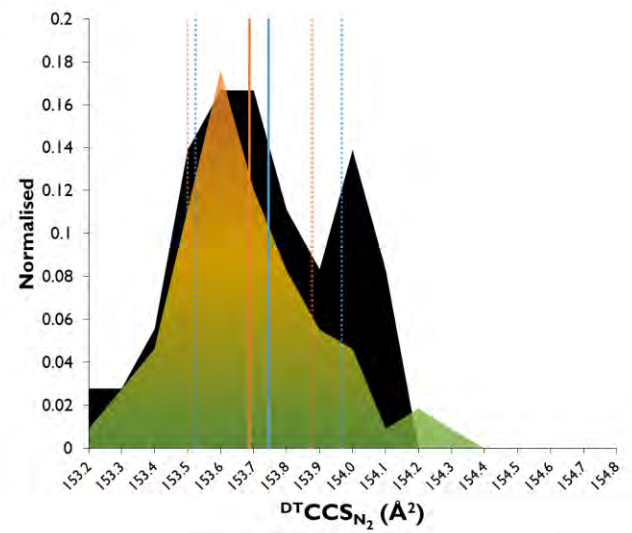
Raw Data (322, +)



L_{eff} Correction Applied



3-Lab Combined Data



- Minor differences in tune modes may reflect higher-order effects (sub-0.5%).
- 3-Lab effective length determined to be **78.236 cm**. This is now applied in the IM Browser Stepped-Field Calculator.
- NB. Single-Field Calculator uses only Agilent Reference System values for calculations.

Interlab Study Results: Measured Values

Stepped-field Approach: Normalised to Agilent Reference System

Positive Ion Mode

Tune Mix Ion	$^{DT}CCS_{N_2}$ (Å^2)	%RSD	Bias (%)
118	121.51 ± 0.21	**0.17%**	**0.17%**
322	153.67 ± 0.20	**0.13%**	**-0.04%**
622	202.67 ± 0.24	**0.12%**	**-0.14%**
922	243.05 ± 0.34	**0.14%**	**-0.24%**
1221	281.25 ± 0.55	**0.20%**	**-0.34%**
1521	315.79 ± 0.81	**0.26%**	**-0.37%**
1821	350.43 ± 1.76	**0.50%**	**-0.23%**
2121	381.40 ± 1.54	**0.40%**	**-0.43%**
2421	410.28 ± 1.49	**0.36%**	**-0.65%**
2721	437.94 ± 1.39	**0.32%**	**-0.74%**

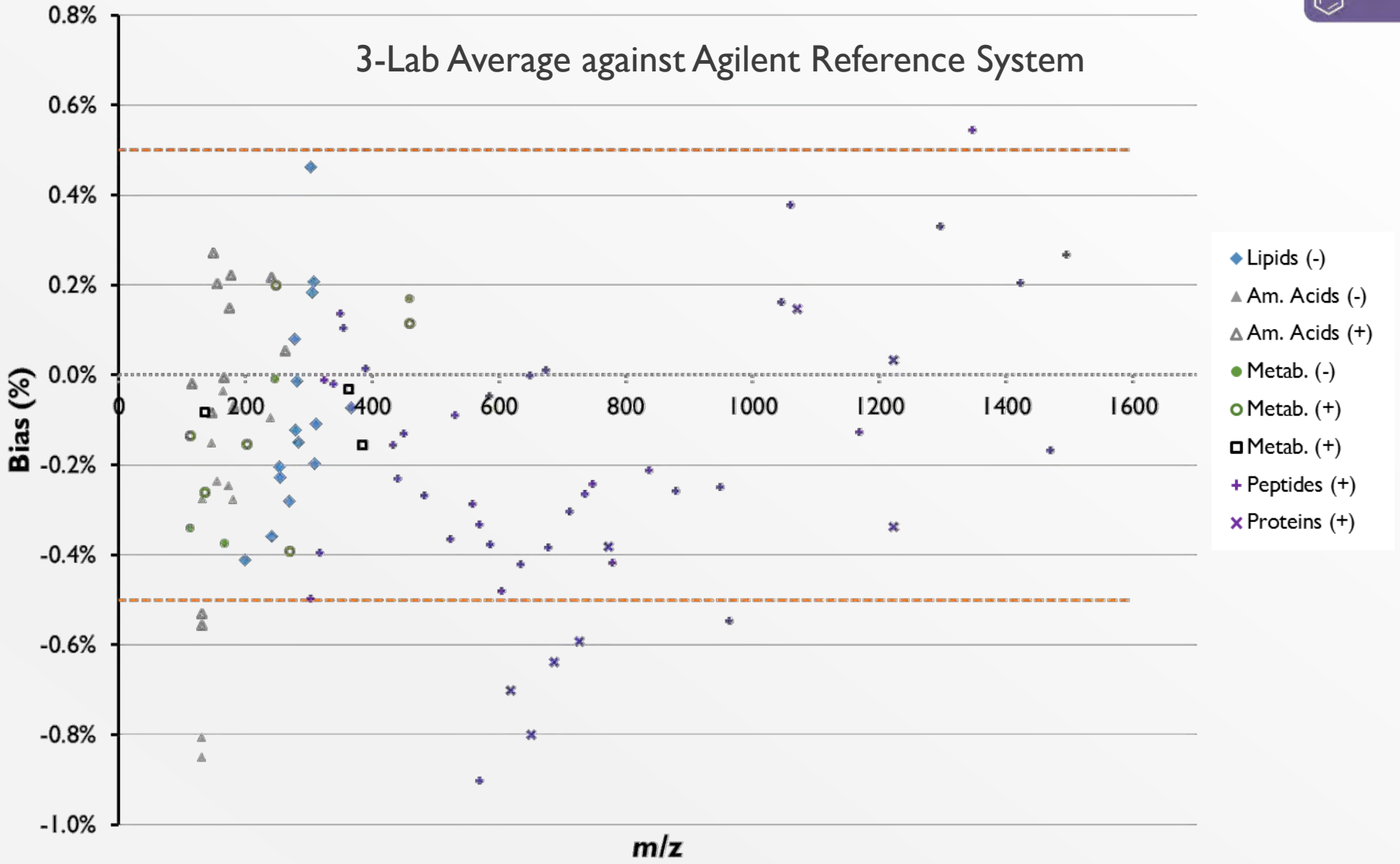
Negative Ion Mode

Tune Mix Ion	$^{DT}CCS_{N_2}$ (Å^2)	%RSD	Bias (%)
112	108.93 ± 0.25	**0.23%**	**0.65%**
301	140.66 ± 0.32	**0.23%**	**0.44%**
601	180.94 ± 0.31	**0.17%**	**0.09%**
1033	255.59 ± 0.53	**0.21%**	**0.10%**
1333	285.29 ± 0.78	**0.27%**	**0.19%**
1633	319.53 ± 1.34	**0.42%**	**0.16%**
1933	354.32 ± 0.64	**0.18%**	**0.50%**
2233	382.39 ± 0.79	**0.21%**	**0.43%**
2533	413.67 ± 1.03	**0.25%**	**0.16%**
2833	431.98 ± 1.12	**0.26%**	**-0.15%**

These data include measurements acquired at 3 international labs under the 4 tune setting options over 3 separate days.

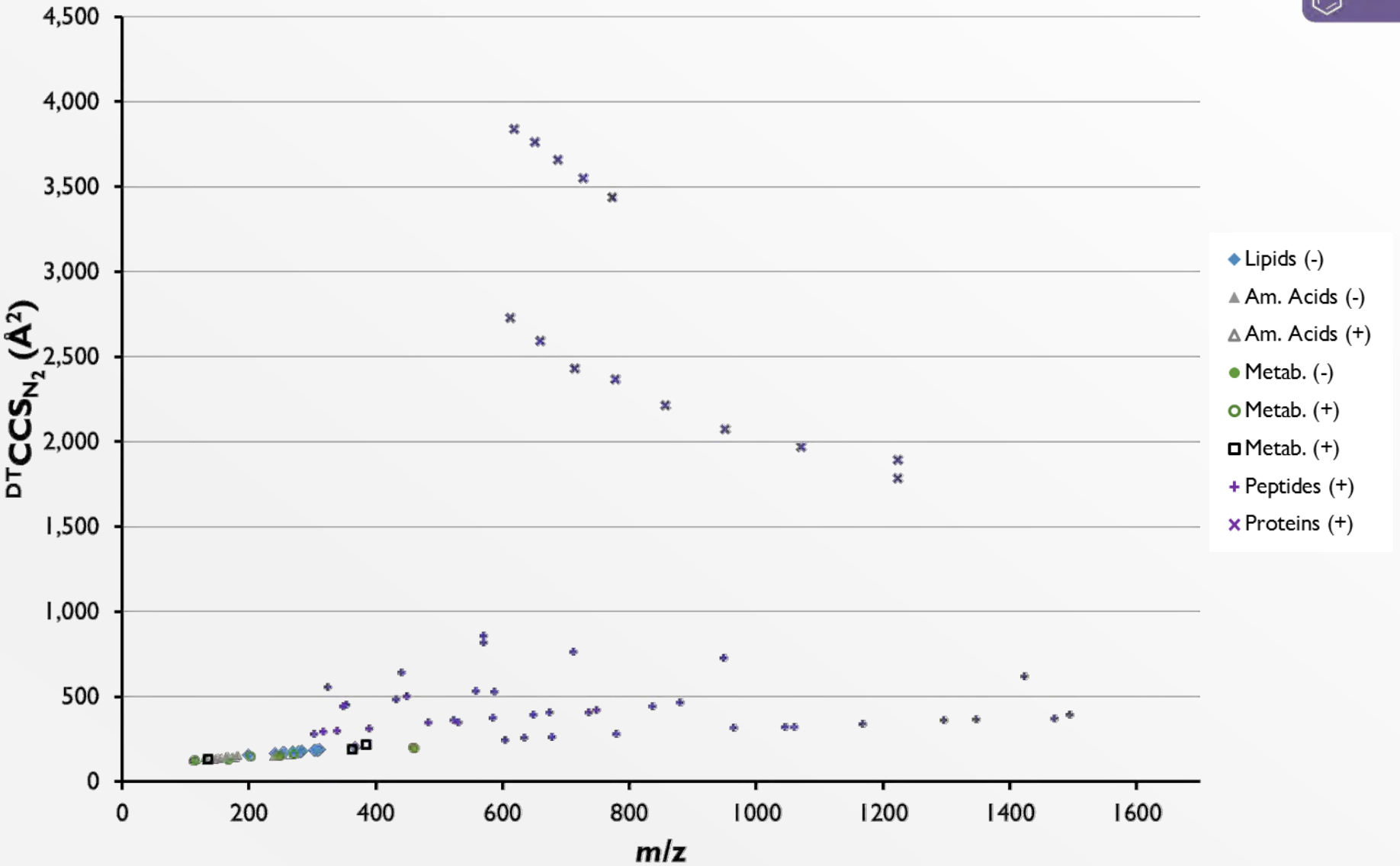
Inter-Lab Results: Stepped-field

Metabolites, Lipids, Peptides, Proteins



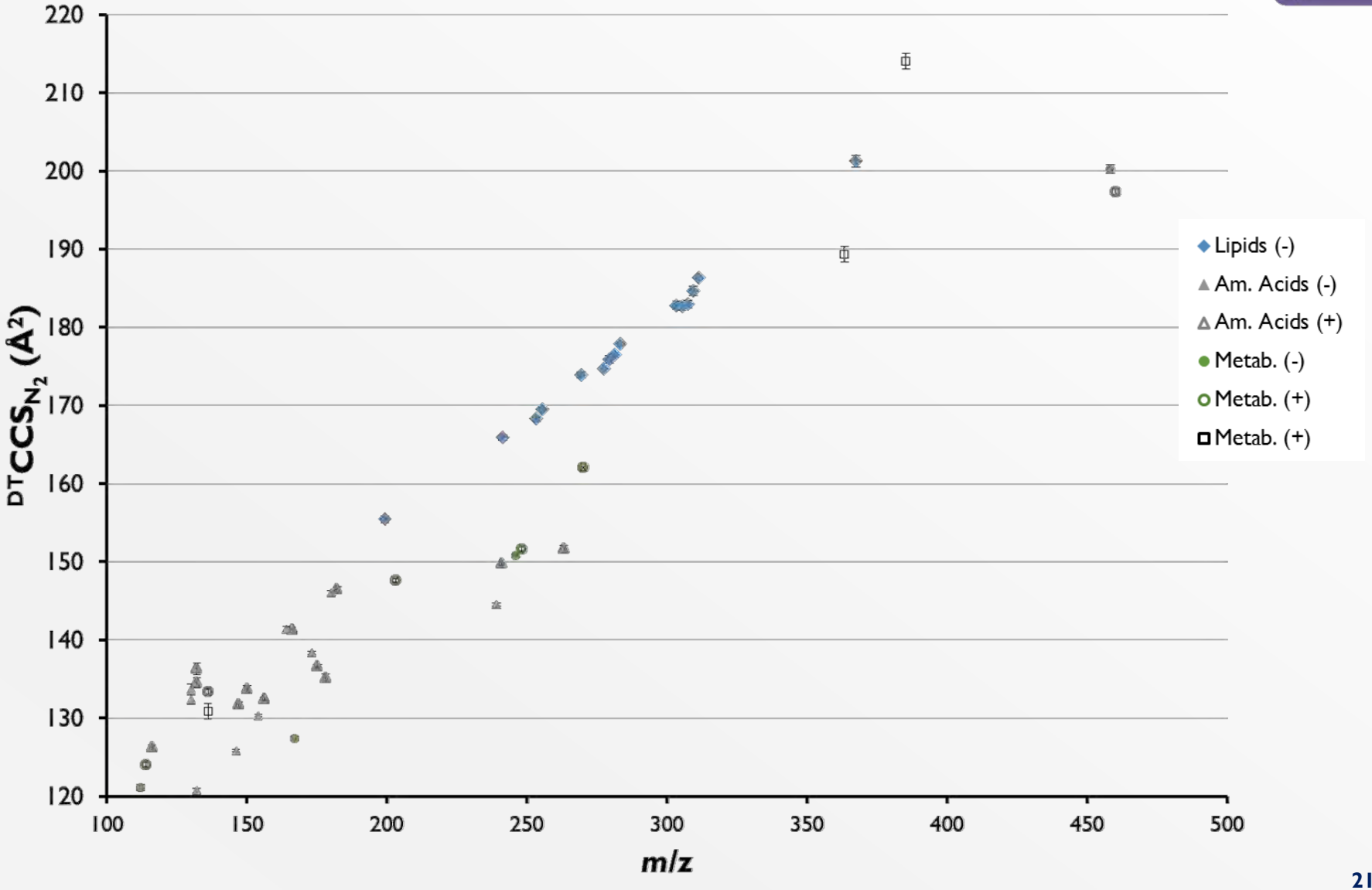
Inter-Lab Results: Stepped-field

Metabolites, Lipids, Peptides, Proteins



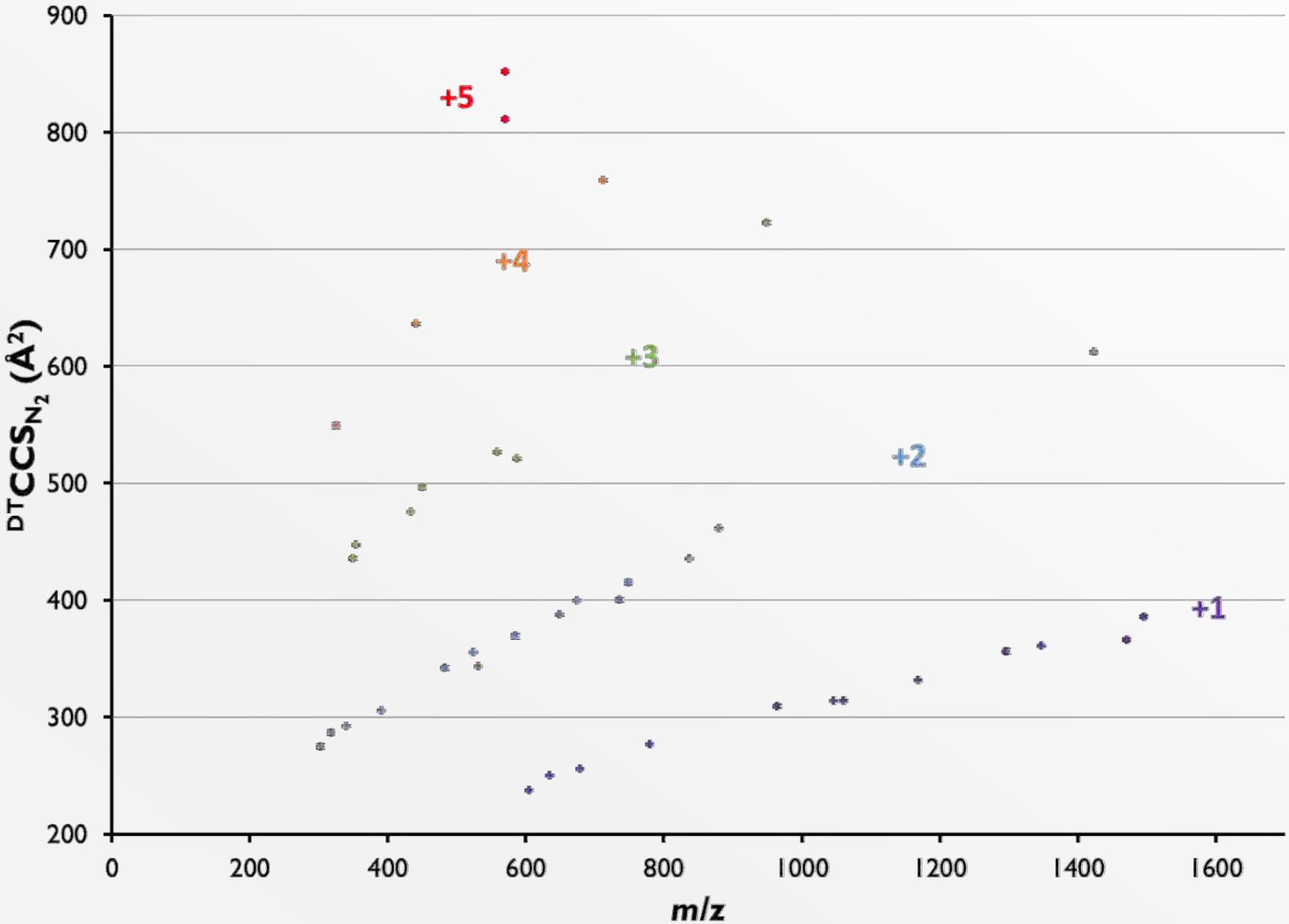
Inter-Lab Results: Stepped-field

Metabolites, Lipids, Peptides, Proteins



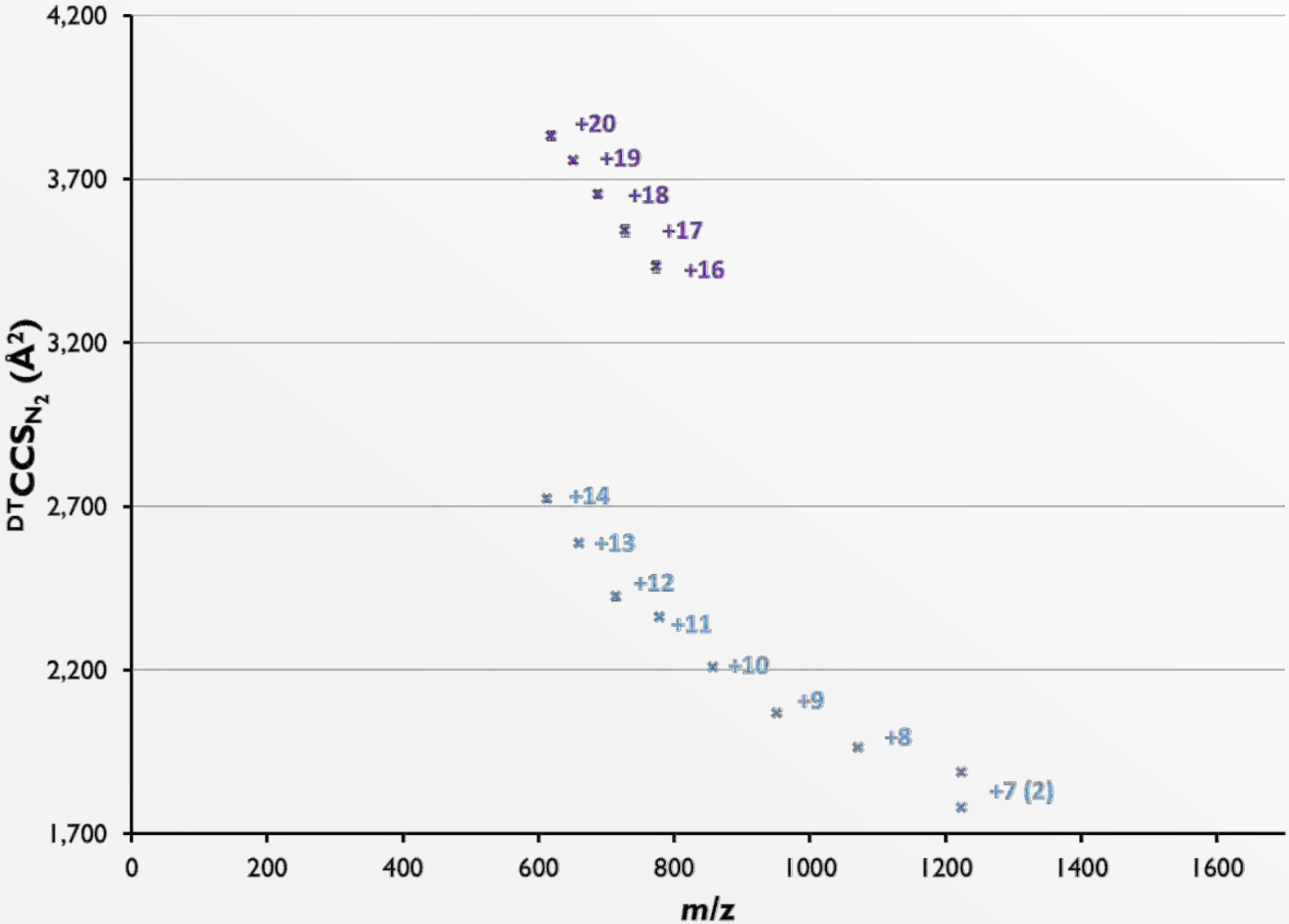
Inter-Lab Results: Stepped-field

Metabolites, Lipids, Peptides, Proteins



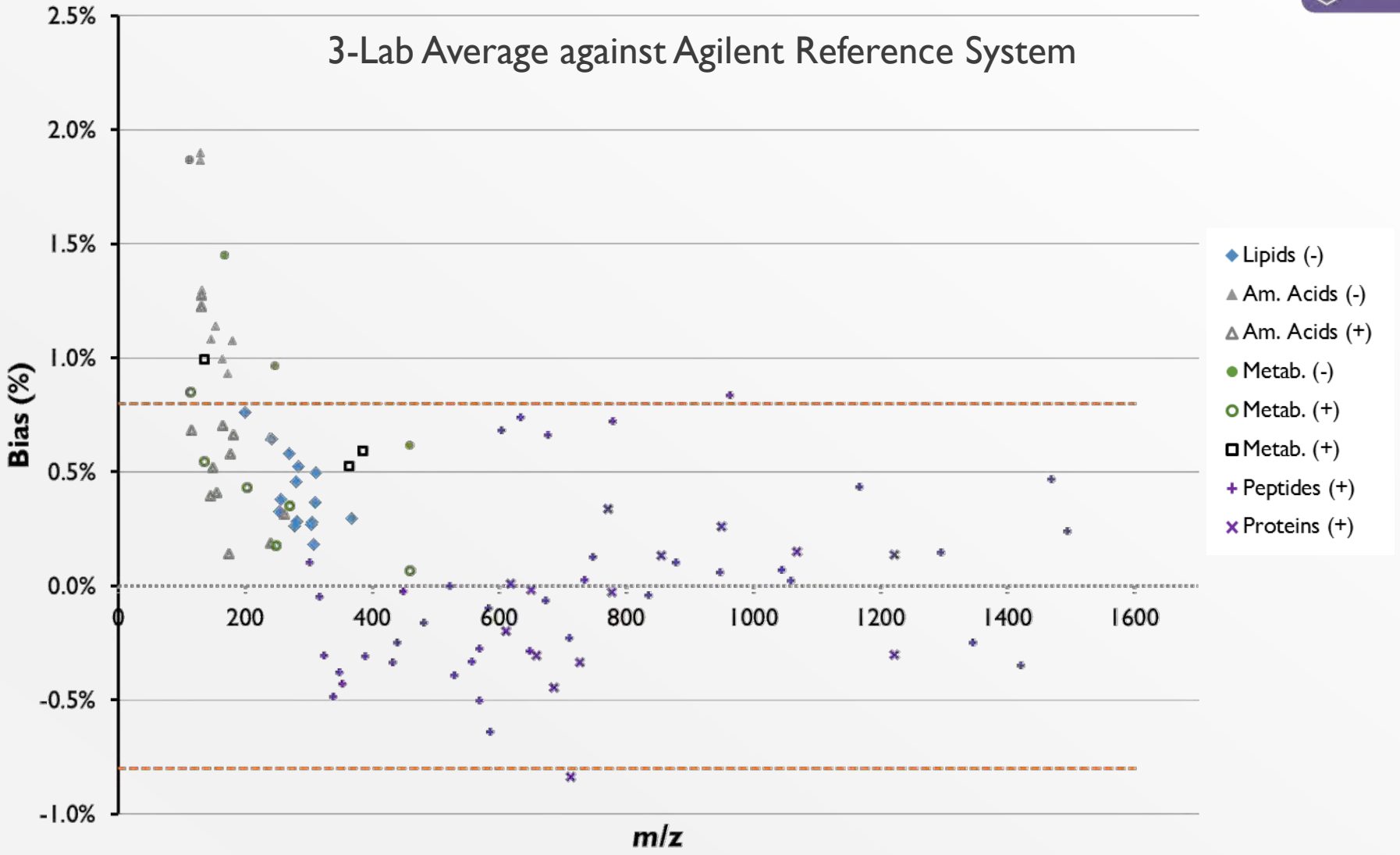
Inter-Lab Results: Stepped-field

Metabolites, Lipids, Peptides, Proteins



Inter-Lab Results: Single-field

Metabolites, Lipids, Peptides, Proteins



Summary: Inter-Lab Study

A Basis for Setting Standards for Independent and Calibrated Operation

Independent (Stepped-Field) ^{DT}CCS Determination

- Single System Precision
  < 0.3% RSD
- Inter-Lab Reproducibility for Tunemix
  ≤ 0.5% RSD
- Inter-Lab Reproducibility for Lipids, Peptides, Proteins and Metabolites
  Mean RSD = 0.30% (3-lab)
  Mean |Bias| = 0.27% (wrt Agilent)

Calibrated (Single-Field) ^{DT}CCS Determination

- Inter-Lab Agreement for Lipids, Peptides, Proteins and Metabolites
  Mean RSD = 0.29% (3-lab)
  Mean |Bias| = 0.31% (wrt Agilent)
- Mean Single-lab |Bias| (Single- vs Stepped-field) = 0.57%
- Publication of method and dataset anticipated for early-2017

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universität wien
Institut für Analytische Chemie

acib austrian center of industrial biotechnology

innovations from nature

INDUSTRIAL PARTNERS

SANDOZ

Boehringer Ingelheim

Lonza

VTU technology

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COMET
Competence Centers for Excellent Technologies

FFG
Austrian Research Promotion Agency

BMWFJ
Federal Ministry for Economy, Family and Youth

BMVIT
Federal Ministry for Transport, Innovation and Technology

SFG
Styrian Business Promotion Agency

Styrian Provincial Government
Economic Affairs and Innovation

zit
Technology promotion agency of the City of Vienna

Standortagentur Tirol

Investigation of Dimeric and Hexameric Halogen-Bonded Supramolecular Capsules by ESI-MS and IM-MS

Ulrike Warzok[1], Lotta Turunen[2], Waldemar Hoffmann[1,3], Kevin Pagel[1,3], Kari Rissanen[2], Christoph A. Schalley[1]

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Introduction

Supramolecular chemistry focusses on the formation of complex molecular assemblies on the basis of non-covalent interactions in order to achieve functionality similar to natural processes. Within this framework, supramolecular capsules have been of particular interest since Rebek published the "tennis ball" capsule[1] in 1993. Numerous examples were introduced making use of diverse binding motives involving hydrogen bonding, metal coordination, ion pair interaction or recently halogen bonding.[2] Hereby, the scope is expanded of both, fundamental understanding and aspired application e.g. in supramolecular catalysis[3]. We herein present the formation of dimeric[4] and hexameric supramolecular capsules based on the interaction of pyridyl-substituted resorcin[4]arene cavitands with positively charged halonium ions by three-center halogen bonds.

Experimental Part

Dimeric and hexameric halogen-bonded complexes were obtained in a two-step procedure by reaction of resorcinarene-based cavitands with silver(I) *p*-toluenesulfonate and subsequently with molecular iodine. Gas phase studies on the complexes were performed with a Synapt G2-S HDMS including ESI-MS, CID tandem MS and travelling-wave ion mobility-mass spectrometry (TW-IMS) experiments as well as with an in-house constructed drift tube IMS instrument. Further characterization of the capsules includes NMR investigation in solution, single crystal X-ray analysis and molecular modelling.

Results and Discussion

ESI-MS gave clear evidence of the selective formation of both, dimeric and hexameric halogen-bonded supramolecular capsules, which exhibit high stability in solution and in the gas-phase. Comparative TW-IMS studies between the halogen-bonded capsules and their silver-coordinated precursors confirm their similar gas-phase structures and the selective, well-defined [N···I^{+}···N] binding mode of the halogen-bonded capsules. Absolute CCS values were determined and compared to theoretical values based on molecular modeling in order to obtain more detailed insight into gas-phase conformation. Combined CID MS/MS-IMS experiments provide detailed information on gas-phase stability, fragmentation mechanisms and characteristics of the fragmentation products. Furthermore, the dynamic behavior of the hexameric halogen-bonded capsules in solution was investigated by comprehensive MS methods.

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Intact Transition Epitope Mapping - A mass spectrometric method for accurate, facile, and rapid identification of specific antibody-peptide reactivities

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Antibodies are indispensable tools for many laboratory techniques and constitute the fastest growing class of medication. As the most important property of an antibody is its capability to specifically recognize its antigen, experimental determination of epitopes is of utmost importance for antibody characterization. We developed a fast and simple epitope mapping method, in which in-solution chemistry is reduced to mixing of peptide and antibody solutions using volatile buffers. The whole antibody/peptide mixture is then electro-sprayed into the gas phase where the unbound peptides (UBPs) are separated from the immune complex in an ion mobility drift cell. The "cleaned-up" immune-complex is subsequently dissociated in the transfer cell and the complex-released peptide (CoRP), the epitope peptide, is identified in the ToF analyzer.

Experimenteller Teil

Anti-hnRNP-A2/B1 mouse IgG2a, anti-His-tag mouse IgG1, and anti-FLAG M2 mouse IgG1 monoclonal antibodies were subjected to buffer exchange using 200 mM NH_4OAc. Protein G´e was digested with trypsin and the His-RA33-A2 protein was digested with LysC/BrCN. Antibody / epitope peptide immune complexes (solutions 3) were formed by direct mixing of synthetic peptides or protein digests (solutions 1) with antibodies (solutions 2) in 1 to 1 molar ratios. 3-5 µl of each solution were loaded into nanoESI capillaries and electro-sprayed (needle voltage 1.3-2 kV) using a Synapt G2S mass spectrometer (WATERS). Solutions 1, 2, and 3 were measured at low (2V) and high (220V) transfer cell energy (TCE) in mobility-ToF mode. IMS-MS/MS data were analyzed using the DriftScope software v.2.4.

Ergebnisse und Diskussion

When solution 1 (FLAG peptide/RA-33 peptide/RA-33 digest/protein G´e digest) was electro-sprayed and exposed to 2V TCE upon separation in the ion mobility cell, singly and multiply charged UBPs were observed. The ion signals lined up along diagonal lines in the arrival-time versus mass-over-charge plots (atomz plots). UBPs were observed with arrival times between 8 and 15 ms for doubly charged and between 15 and 22 ms for singly charged ions. By contrast, when the collision energy in the transfer cell of the mass spectrometer was elevated up to 220V TCE, the ion signals of the intact peptides completely disappeared due to harsh fragmentation and only a "cloud" of fragment ion signals with low *m/z* values were observed, all with arrival times of their precursors.

When the mixtures consisting of the antibodies and the peptides (solutions 3) were electro-sprayed and exposed to 220V TCE, only one or a few singly and/or doubly charged ion signals were observed in the atomz plots with arrival times that corresponded to the arrival times of the multiply charged antibody ions or their fragments (ca. 20-25 ms; see solutions 2). These longer drift times of the antibody-released peptide ions (CoRP ions) are explained by the in-solution formation of the non-covalent immune-complexes and, upon their transitions into the gas phase, their migration through the ion mobility cell as intact immune-complexes.

Here, UBPs are separated from the immune-complex ions. Subsequent release of the “cargo” of the antibody in the transfer cell enables mass determinations of the intact peptides by ToF MS analysis, directly identifying the epitope peptides.

The following rules apply: (1) CoRPs, unlike UBPs, possess drift times that match with the drift times of the antibody ions. (2) CoRPs, unlike UBPs, survive the fragmentation conditions in the transfer cell and are detected as intact, i.e. un-fragmented, peptides.

Neue Aspekte

This is the first report on gas phase epitope mapping through which epitopes are accurately identified in a single experiment.

Formation and Properties of a Compact Protein Unfolding Intermediate in the Gas-phase

Knut Kölbel and Frank Sobott

Introduction:

Collision-induced dissociation (CID) is best known as an activation technique for obtaining sequence information of e.g. peptides in *bottom-up* strategies or, more generally, to confirm the identity of a given analyte. Ions are accelerated and collide with a stationary gas with the kinetic energy being converted to thermal energy. The increased molecular ions' internal energy results in the mobilization of protons and, finally, bond dissociations.

In Native-MS, CID is used less "disruptively" for purposefully dissociating non-covalent protein complexes (stoichiometry determinations). When CID is applied to monomeric proteins, intramolecular folds are driven apart instead of intermolecular interfaces. In combination with ion mobility this approach is increasingly used for CIU (Collision-induced unfolding) measurements in structural biology, examples of which are reported here.

Experimental:

Most measurements were done with a monomeric two-domain protein, D-alanine:D-alanyl carrier protein ligase (DltA, ≈ 56 kDa). Following a pre-incubation with or without ATP or AMP being present, DltA was sprayed from home-made gold-coated borosilicate emitters. Mass spectra and arrival time distributions (ATDs) were recorded in an ESI Q-ToF Synapt G2 HDMS with ETD (Waters) upon nano-electrospray ionization (nanoESI) according to standard procedures [1]. Briefly, mass spectra and ATDs of precursor and activated ions (MS/MS) were recorded with increasing trap cell collision energies with the other settings remaining constant. Approximate values of collision cross sections (CCSs) were obtained by external calibration and compared to theoretical ones obtained by the projection approximation method.

Results:

DltA catalyzes the ATP-dependent formation of an D-alanyl-AMP intermediate. Based chiefly on computational modeling, a catalytic cycle has been proposed for this reaction, which involves some conformational rearrangements of the *C*-terminal domain of DltA [2]. Our original interest had been aimed at characterizing hypothetical conformations of free DltA; comparable to those of ligand-bound protein. However, when sprayed from neutral buffers, ionization of DltA, regardless of its ligand binding state, yields lowly-charged (+9 to +12 and +12 to +15, from 100 mM triethylammonium or ammonium acetate, respectively) and – somewhat surprisingly – "overly compact" molecular ions.

The ATDs corresponding to each charge state proved broad and asymmetric. Increased collision energy resulted in slight shifts of peak maxima (i.e. drift times and, hence, the CCSs) and drastic peak shape alterations below the peaks' half height. Because the major effect thus occurred in the lower half of the peaks, the notion of the peak width (at half height!) as an indicator of conformational ***flexibility*** proved largely inapplicable. Rather a mixture of slightly differing sub-species (i.e. conformational ***heterogeneity***) resulting in a set of redundant and merging peaks was considered. This was proven by systematic activation (5-150V) of each accessible charge state (+10 to +15) and thorough peak deconvolution of the obtained ATDs. Additionally, a clear sequence of unfolding steps could be established.

Compared to well-known "standard" proteins, the stability of the DltA-ligand complexes, also at high collision energies, is considerable with ligands being retained also by conformationally extended (i.e. denatured) protein. While "global unfolding" was not affected at all by ligand binding, the sub-species distribution within the compact ensemble was clearly affected. This extends to the putative activation barriers between the different unfolding intermediates. Currently this study is being extended with respect to basic mechanistic questions (e.g. barrierless, "downhill" vs. thermodynamically controlled reaction).

References:

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New Aspects:

As opposed to accepted wisdom, multistep-CIU does not necessarily imply domain-separated unfolding.

Differentiation and relative quantification of chondroitin sulfate isomers by ion mobility spectrometry-mass spectrometry and pulsed-field gradient NMR

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Einleitung (120 Wörter)

Glycosaminoglycans (GAG) such as chondroitin sulfate (CS) are important constituents of the extracellular matrix and play an important role in all vertebrates [1].

MS/MS (subsequent to enzymatic digestion) is normally utilized to differentiate the naturally occurring isomers (4- and 6-sulfate) of CS. Qualitative and semi quantitative evaluation of the MS/MS results requires standards to compensate the different ionization potentials of the CS isomers and to determine the most relevant fragments [2].

We were looking for alternative methods which enable the differentiation of GAG isomers without the need of using MS/MS - particularly regarding the future analysis of artificially sulfated, more complex GAG-derivatives. For this purpose, isomeric CS disaccharides obtained by chondroitinase ABC digestion served as the compounds of interest.

Experimenteller Teil (120 Wörter)

Two commercially available CS disaccharide standards and one sample obtained by digestion of the CS polysaccharide with chondroitinase ABC were investigated via ion mobility mass spectrometry (IMS) and nuclear magnetic resonance (NMR) spectroscopy.

Mass spectra were acquired on a TOFWERK IMS-TOF which has been essentially described in [3]. Analytes were ionized by ESI. Nitrogen was used as the drift gas at atmospheric pressure and a temperature of 30°C.

The proton NMR spectra were recorded at 25°C using an inverse 5 mm probe on a Bruker 600 MHz NMR-Spectrometer. Diffusion measurements were performed at 37°. All samples were investigated as about 5 mg/ml solutions in D_2O.

Ergebnisse und Diskussion (300)

The negative (deprotonated form at *m/z* 458) and positive (triply sodiated disaccharide at *m/z* 526) ion mobility mass spectra of the digested CS show two signals which are even baseline-separated in the case of the positive ion mode. The IMS-MS spectra of CS standards verify that the first peak, characterized by a shorter drift time, represents the 4-sulfate and the second peak the 6-sulfate.

These findings could be confirmed by ^{1}H pulsed field gradient (PFG) NMR spectroscopy [4]. The logarithmic plot of I/I_0 in dependence on the applied field gradient strengths shows different slopes for the CS isomers. The signal intensity of the resonance assigned to the C4S

isomer decays faster, corresponding to a lower apparent self-diffusion coefficient than the C6S isomer.

These data are in excellent agreement with the IMS-MS results. In a nutshell, the CS isomer which is sulfated at the C4-position is “faster” than the C6S-form in both environments, i.e. in the gas phase as well as in solution, caused by the conformational differences between the two isomeric forms.

The relative quantification by means of IMS-MS gave different results in positive and negative ion mode which could not be explained by an insufficient baseline separation alone. The comparison of the obtained relative moieties with the results of MS/MS and standard 1H NMR measurements provided evidence of different ionization efficiencies of the two isomers in the negative but no significant differences in the positive ion mode.

All in all, the differentiation and relative quantification of the two GAG disaccharide isomers in mixture is possible by IMS-MS in the positive ion mode without the need to perform MS/MS experiments. Additionally, purified reference compounds are not absolutely needed.

Referenzen (max 5 Stück)

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Neue Aspekte (20 Wörter)

IMS-MS combined with (PFG) NMR allows differentiation, relative quantification and structural identification of CS isomers in mixtures without purified standards.

Stichworte

Chondroitin Sulfate; Disaccharide; Ion Mobility Spectrometry-Mass Spectrometry; NMR; Apparent Self-Diffusion Coefficient.

Pyrylium-based dye and charge tagging in proteomics

Malte Bayer and Simone König

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Introduction

The pyrylium group has been established as a selective reagent for ε-amino groups in proteins. Especially for fluorescence labeling it offers numerous advantages over traditional NHS-ester chemistry such as the small size of the fluorophore leading to reduced spot shifts in 1D- and 2D gel electrophoresis[1, 2]. But even though pyrylium-based fluorescent modifiers have been around for more than a decade, they have not been explored to their full capacity as of yet. In an effort to determine their specificity and potential side products we used mass spectrometry (MS) to study exemplarily peptides containing no, one, and two lysine residues and either one or no cysteine residues. They were labeled with Lightning Red (LR), a dye containing pyrylium functionality[3].

Experimental part

LR and dimethylformamide (DMF) were supplied by Serva Electrophoresis GmbH. [Glu1]-fibrinopeptide B (GFP), Substance P and sodium bicarbonate were purchased from Sigma-Aldrich. Transthyretin peptide SKCPLMVK was synthesized by ThermoFisher. MeOH came from Fluka, dithiothreitol (DTT) from Applichem.

For labeling, peptides were dissolved in 8 µL $NaHCO_3$ (5 mM, pH 9.3) with 10 mM DTT and incubated for 15 min at room temperature. Then 40 µL of MeOH and 5 nmol of LR in 1.97 µL anhydrous DMF were added and the solution was incubated for 2 h at 50°C in an ultrasonic bath (yields >30%).

MS was used to investigate the reaction products (Q-TOF Premier, Waters Corp.). Samples were supplied either by liquid chromatography (nanoAcquity) or by manual nanospray.

Results and discussion

Peptide labeling proceeded at 2h in a high content of organic solvent (84 %). Gas phase fragmentation proved both labeling of lysine residues as well of that of the N-terminus though at lower intensities. Labeling of other amino acids was not abundant but. one side reactions was a rearrangement of the labelled N-terminus with an adjacent glutamic acid in case of GFP. Nominal additions of 158, 173, 215, 303, and 441 Da in low intensities were also observed. As pyrylium-labeled amines are acid labile and the mobile phase contained 0.1 % formic acid neither decomposition nor gas phase reactions can be ruled out as a source for these modifications.

Interestingly, for N-terminally labeled peptides a- and b-type ion series were detected predominantly. Therefore, LR may also be used for charge tagging of peptides as an alternative to the commonly used quaternary ammonium[4] and phosphonium salts[5]. Charge tagging improves sequence assignment and sensitivity due to simplification of fragmentation spectra. Conclusively, pyrylium-based modifiers have a high potential in protein and peptide analysis for their specificity, few side reactions, fluorogenic and chromophoric properties (reaction product is colored red), as well as the potential use as a charge tag.

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An Integrated Workflow for Structural Proteomics Studies based on Cross-linking/Mass Spectrometry with an MS/MS Cleavable Cross-linker

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Novel aspects: Integrated workflow for a comprehensive, robust, and automated analysis of cross-linked products using MS-cleavable cross-linkers.

Cross-linking combined with mass spectrometry (MS) has evolved as an alternative strategy in structural biology for characterizing three-dimensional structures of protein assemblies and for mapping protein-protein interactions. In this work, we systematically evaluate the different fragmentation methods available on an Orbitrap Fusion mass spectromete, namely CID, HCD, ETciD, and EThcD, with the aim of optimizing the automated identification of cross-linked peptides. Our strategy is validated for cross-linking three proteins, ß-lactoglobulin, bovine serum albumin (BSA) and the tetrameric tumor suppressor protein p53. Additionally, we tested our workflow for analysis of an *E. coli* cell lysate. For data analysis, the *in-house* software MeroX is employed, providing the basis for a robust and reliable automated assignment of cross-linked products [1].

BuUrBu [2] was added in 50-fold molar (for p53) or 100-fold molar (ß-lactoglobulin, BSA) excess. *E. coli* cell lysate (1mg/ml) was cross-linked with 5mM BuUrBu, reactions were quenched after 120min (4°C). *In-solution* digestions were performed with trypsin or GluC/trypsin (for p53).
Samples were analyzed by Nano-HPLC/Nano-ESI-MS/MS on an U3000 RSLC system (RP-C18, 75µM×250 mm, 2µm, 100Å) coupled to an Orbitrap Fusion (ThermoFisher Scientific). 90min gradients were applied

for single protein analysis, 300min for *E. coli* cell lysate. Data were acquired in data-dependent MS/MS mode. For stepped HCD and ETD-based methods, two precursor selection modes were employed, (i) top 5sec/most intense and (ii) highest charge, charge states >2 were selected for fragmentation. Cross-linked products were analyzed with MeroX 1.6.0 [1].

The basis of this study is the use of an MS/MS cleavable cross-linkers, such as BuUrBu [2], for an automated assignment of cross-links based on characteristic reporter ions.

On the basis of a thorough comparison of different fragmentation techniques available on an Orbitrap Fusion mass spectrometer, we propose an integrated workflow for a comprehensive, robust, and automated analysis of cross-linked products. The use of MS/MS cleavable cross-linker presents a large step toward a reliable assignment of cross-linked products as specific fragment ions are generated under tandem MS conditions. Considering the *per se* higher number of identified cross-links in stepped HCD experiments, mainly due to the higher number of MS/MS spectra recorded, this fragmentation technique should be favored over EThcD. The major aim should be to maximize the number of cross-links in one single LC/MS/MS analysis. The obvious strength of our MS/MS cleavable BuUrBu-linker is that the characteristic doublets of the cross-linker as well as backbone fragments of the connected peptides are already observed at the MS/MS level. As MS^3 experiments are not required for a cross-link assignment, our workflow is applicable to every lab with access to a high-resolution mass spectrometer with tandem MS capabilities, such as Q-TOF or Q-Exactive Orbitrap mass spectrometers. For single proteins and protein complexes our workflow performs with high confidence, scoring cross-links with an FDR above 0.5%. In case whole proteomes are investigated, prefractionation and enrichment steps are required for a confident assignment of cross-links.

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Absolute quantification of core histones in zebrafish embryos by MS Western

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Despite numerous application pitfalls and technical limitations (1), Western blotting (WB) is still preferred over mass spectrometry for the quantification of a limited selection of biologically interesting proteins. Here we report on a method of multiplex absolute quantification of proteins termed the MS Western that accurately determines the absolute (molar) content of dozens of user-selected proteins at the low femtomole level in whole cell/tissue lysates with no requirement for their metabolic/chemical labelling or antibodies. MS Western outperformed WB by the protein detection specificity, linear dynamic range and sensitivity of protein quantification. We employed MS Western to quantify core histones: H2A, H2B, H3 and H4 in ten early stages of zebrafish embryogenesis and revealed unexpected trends in their molar abundance and stoichiometry

Experimenteller Teil

MS Western effectively merges the three established analytical approaches: GeLC-MS/MS (2); proteotypic peptide clubbed with “top N peptides” protein quantification (3,4) and QCAT (5) like synthesis of isotopically labelled chimeric protein (CP) encompassing the sequences of proteotypic peptides from target and reference proteins (e.g. BSA).To quantify proteins of interest the gel slab approximately matching the Mr of target proteins were excised and co-digested with bands of the CP and of the reference protein. The recovered tryptic peptides were analysed by LC-MS/MS and the molar quantity of each target protein was inferred from the molar content of the CP, which in turn was referenced to the known amount of the BSA.

Ergebnisse und Diskussion

Absolute quantification of proteins in moles opens up the attractive possibility to determine the stoichiometry of subunits of protein complexes, protein abundances within pathways, as well as molar ratios of proteins to non-proteinous molecules, such as DNA. We employed MS Western to determine the molar content of H2A, H2B, H3 and H4 in zebrafish embryos over ten developmental stages from 1-cell stage to Shield stage. Since MS Western determined the molar content of individual histones, we expressed it as the number of molecules per embryo and related it to the histone content required to pack the genomic DNA. At the 1-cell stage histones are present in 5000-fold molar excess than actually required to pack the genomic DNA into nucleosomes, which it dwindles down to 13-fold excess at the later 1000-cell stage. At the very early stages the histones stoichiometry deviated from the expected equimolar ratio, which was more closely approached at the later stages. H3 (and, to lesser extent, also H4) histones were consistently present in the higher amount compared to H2A and H2B. At the same time, the content of H2A and H2B was remarkably stable and close to the expected equimolar stoichiometry, which supports the notion that they form a stable dimer within the nucleosome.

Neue Aspekte

Simple, inexpensive and accurate absolute quantification of proteins directly from cell or tissue lysates

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ArgC-like digestion: complementary or alternative to tryptic digestion?

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Enzymatic digestion of complex protein samples is often performed by use of multiple proteases to improve protein identification and characterization. [1] Combining trypsin with ArgC is one option to enhance sequence coverage in bottom-up proteomics. However, the low selectivity of this endoprotease impairs the benefit of the combination. [2] Our approach here is to mimic ArgC digestion by chemically modifying all lysine residues in proteins so that trypsin can only cleave C-terminal to arginine. Four different amine modifications, dimethylation, acetylation, propionylation [3] and carbethoxylation were tested and the protocols were optimized. The different protocols were applied to a complex protein sample (Escherichia coli) and the protocol with the best results was finally compared to a conventional tryptic digestion.

Experimenteller Teil

Proteins were bound to the NHS Mag sepharose beads (GE Healthcare) according to the supplier's protocol

Propionylation. 480 µL methanol and 120 µL TEAB (Sigma Aldrich, 1.0 M, pH = 8.5) were added to the immobilized proteins. Before adding 6 µL propionic acid anhydride (Sigma Aldrich) the bead suspension was cooled down to 4°C. After 2 hours of incubation at 4°C the reaction was stopped.

The washed protein carrying beads (1000µg) were suspended in 90 µl 50mM TEAB and 10 µg of trypsin was added for overnight digestion at 37°C.

MS measurements of single protein digests were performed with a MALDI TOF/TOF Analyzer (ABI 4800, Applied Biosystems) and LC-MSMS of complex samples were performed on Thermo Scientific™ Q Exactive.

Ergebnisse und Diskussion

In the beginning the modification protocols, which show satisfying results on peptide level, had to be optimized on protein level. A nearly complete conversion of the primary amines was achieved for all modifications. Applying those optimized protocols on a more complex sample (Escherichia coli) reveals that modification with propionic acid anhydride prior digestion with trypsin leads to the best results indicated by the highest number of identified peptides and proteins. Additionally the highest complementarity to a tryptic digestion was observed for this reagent. Comparing the ArgC-like digestion using propionic acid anhydride to a conventional tryptic digestion reveals that both methods are comparable to each other and unexpectedly in many assessed parameters the ArgC-like results are even superior. The main reasons for the superiority of ArgC-like digestions are a higher number of identified proteins, a lower occurrence of peptides with missed cleavages and higher average ion scores which result in a higher proteome coverage, higher cleavage and fragmentation efficiency. It is therefore concluded that the Arg-C like digestion should no longer be regarded as a complementary approach, but forms a viable and superior alternative to the conventional trypsin digestion.

Neue Aspekte

Introducing alternative strategy to a conventional tryptic digestion.

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Proteome-wide detection of proteolysis in blood plasma by the SDS-PAGE-migration profile

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Many physiological processes are regulated by proteases, where proenzymes undergo proteolytic cleavage releasing the active enzyme. For example, Factor XII is proteolytically activated when in contact with negatively charged surfaces, starting coagulation and inflammation. Kwiatkowski et al. developed a method to demonstrate proteolytic activity in tissue extracts. The extracted proteins are separated by SDS-page. Each of the obtained lanes are cut into consecutive bands and analyzed by bottom-up proteomics. The LC-MSMS data is used to calculate migration profiles for each protein, where the relative amount is plotted against migration distance (kDa) in the SDS-page[1]. Here we studied the activation of Factor XII.

Experimenteller Teil

Human plasma was activated by dextran sulfate (DXS) or inorganic polyphosphate (polyP). An immunoprecipitation was performed on the activated plasma samples and a non-activated control sample. Samples were pre-cleared with protein G sepharose beads followed by incubation with anti-FXII antibody-coated protein G sepharose beads. The obtained eluates were loaded onto a 10% SDS-page. Each of the obtained bands were cut into 19 consecutive pieces that underwent in-gel-tryptic digestion and LC-MS/MS analysis (Dionex Ultimate 3000 nano-UPLC coupled to an Orbitrap Fusion, Thermo). Migration profiles of all identified peptides were obtained by plotting their areas under the curves (y-axis) against the molecular weights of the corresponding bands in the SDS-page (x-axis).

Ergebnisse und Diskussion

The obtained migration profiles show a distinguished pattern for the FXII peptides in plasma activated with polyP and DXS. When plasma is activated by DXS, the migration profile of FXII shows a clear separation of the heavy chain from the light chain. This separation is not observed in the case where plasma was activated by polyP. These results corroborate previous findings by Engel et al. that suggest activation of FXII by polyP as a result of conformational changes rather than by cleavage at the activation site (R353-V354) [2]. These findings might provide an explanation for FXII activation by polyP resulting in coagulation and activation of the kallikrein-kinin system, whereas by DXS only activates the kallikrein-kinin system [3]. The method presented in this work showed to be a useful tool to understand the differences in the activation of FXII by different negatively charged molecules.

Neue Aspekte

SDS-PAGE-migration-profiles can be applied on a wide array of biological systems, where proteolytic events have to be investigated proteome wide.

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Glycan Fingerprinting using Cold-Ion Infrared Spectroscopy

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Oligosaccharides are of great importance for a variety of biological functions such as cell-cell-recognition, immune response or protein folding. However, compared to proteins or DNA, oligosaccharides are not assembled in a linear, template-derived fashion. Instead they are synthesized by a complex biological machinery, which leads to branched structures with a diverse regio- and stereochemistry. The analysis of the resulting isomers is usually very challenging and typically involves a combination of sophisticated chromatography, mass spectrometry and ion mobility mass spectrometry steps. Here we show that cold-ion gas phase infrared spectroscopy is a very promising alternative for the in-depth structural analysis of complex oligosaccharides.

Experimenteller Teil

The experimental setup consists of a mass spectrometer that is connected to the FHI IR free-electron laser and equipped with a source for superfluid helium droplets. Molecular ions are generated using nESI, mass-to-charge selected, and accumulated in a linear ion trap. Superfluid helium droplets are subsequently guided through the trap where they can pick up ions, which are rapidly cooled to the internal temperature of the droplet (0.37 K). While the droplet itself is optically transparent, irradiation with intense, narrow-bandwidth IR radiation can lead to the ejection of ions from the droplet if the wavelength is resonant with a vibrational excitation of the ion. Monitoring the ejection efficiency as a function of the wavelength yields IR spectra of ultra-cold ions.

Ergebnisse und Diskussion

In order to assess the potential of cold-ion spectroscopy for oligosaccharide analysis, IR spectra of a series of synthetically derived mono-, di- and trisaccharide standards were recorded. For each of these oligosaccharides, unique and highly diagnostic absorption patterns with a variety of well-resolved bands was obtained. In some cases, the line-width in the spectra was equal to the corresponding bandwidth of the laser radiation (FWHM $\approx$ 4 cm^{-1}). This unprecedented resolution reveals remarkable differences in the overall IR signatures and allows a simple, fingerprint-based discrimination between isomers, even if they merely differ in the stereochemistry of a single OH group.

Next, we extended the scope of our analysis from synthetic standards to naturally occurring glycans. To do so, the isomeric blood group related antigens Lewis b and Lewis y, as well as the tetrasaccharide isomers lacto *N*-neotetraose and lacto *N*-tetraose from milk were investigated. Also for these samples, well-resolved and highly diagnostic absorption features were obtained which allows their unambiguous discrimination.

Taken together, our data reveal that cold-ion spectroscopy has the potential to overcome all the challenges previously encountered in oligosaccharide analysis. Its unprecedented resolving power provides highly diagnostic absorption patterns—a spectral fingerprint that is unique for each oligosaccharide. For larger glycans, the variety of fragments obtained by sequential MS also enables a fragment-based fingerprinting. These spectra can be stored in databases to provide reference data for quality control or serve as increments for the identification of unknown samples. As such, cold ion spectroscopy has the potential to serve as the ultimate analytical tool to fully disentangle the detailed structure of oligosaccharides and might prove an enabling technology for the glycosciences.

Neue Aspekte

In-depth structural analysis of oligosaccharides using gas-phase IR spectroscopy

The Usage of Direct Inlet Probe in combination with High Resolution Mass Spectrometry for the Characterization of Heavy Petroleum Products

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Power-function Resolution Filter in Fourier Transform Mass Spectrometry

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Abstract: Fourier Transform of time domain acquisitions in FT-ICR-MS produces frequency domains, which contain frequency signals of sine cardinal (sinc) shape surrounded by sinc wiggles. These wiggles represent artifacts of the FT-result in the frequency, which originate from the time-domain truncation of the detection signal within the acquisition of the superimposed sine waves of the cyclotron frequency data. A new filter is developed to identify and remove these wiggles from both frequency and mass spectra. The newly developed filter is based on distinguishing between the FWHM of the correct frequency/mass signals and the FWHM of their corresponding wiggles. The filter draws a reliable confidence limit of resolution range, within which a correct frequency/mass signal is identified. The filter is applicable over a wide mass range of metabolic interest (200-800) amu.

Development of an autarkic desorption electrospray ionization source for in-field DESI-MS applications

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Introduction

The ambient ionization method desorption electrospray ionization (DESI) combined with mass spectrometry (MS) is a capable tool for the analysis of various samples.[1,2] It allows direct surface sampling under atmospheric pressure conditions without any previous sample preparation. The simple and fast measurement procedure allows for high sample throughput [3] and is easy to handle. These characteristics predestinate DESI for in-field measurements. Due to its need for pressurized gas, high voltage and a solvent source, DESI-devices are currently bound to laboratory sites. We developed a self-sustaining and user friendly DESI-source to facilitate direct analysis at the sampling site. The source can be used with miniaturized portable mass spectrometers as well as with lab-based devices.

Experimental

MS measurements were performed with a miniaturized ion trap mass spectrometer (Mini 11, Purdue University, West Lafayette, USA)[4] and an orbital trapping mass spectrometer (Exactive, Thermo Fisher Scientific GmbH, Bremen, Germany). The new autarkic DESI-source was operated with 6 bar of atmospheric air, 4 kV spray voltage in positive ion mode and a solvent flow rate of 5 µl min^{-1} of a methanol water mixture (9:1) with 0.5 % formic acid. The sample-to-sprayer distance was 1-2 mm and the distance between the sprayer and the MS inlet was about 5 mm. The angle between the sample surface and the solvent spray direction was 60°. Measurements in front of the Exactive Orbitrap were realized with a home-built 48 cm long transfer-capillary.

Results and Discussion

The new DESI-source consists of an upside-down mounted DESI-sprayer below a slit in a sample table. During the measurement, the spray is directed upwards through the slit onto the bottom side of the sample object. The slit in the sample table is oriented coaxially with respect to the ion transfer capillary of the atmospheric pressure interface (API) of the mass spectrometer. A *x,y*-translation stage combined with a rotation stage allows for precise positioning of the sprayer-to-sample and sprayer-to-transfer-capillary geometry. The sample table works as a flat sample holder which protects the sensitive sprayer capillary from damage/contamination by sample objects. Moreover the sample holder determines the geometry for consecutive measurements or different samples and consequently improves the reproducibility of measurement conditions. A source-integrated

compressor delivers 6 bar of filtered environmental air to assure stable DESI-source operation. Via a pressure bypass a pressure pump supplies the sprayer with solvent. With a controllable pressure system connected to the pressure pump the flow rate can be adjusted continuously between 1 and 50 µl min^{-1}. The adjusted flow rate is monitored in real time with an implemented flow sensor and the related software. The whole system is powered by a rechargeable battery and allows for a continuous runtime of about 3 hours. Comparative measurements with the new DESI-source connected to either the miniaturized mass spectrometer Mini 11 or a high mass resolution benchtop Exactive Orbitrap instrument demonstrated good working quality. Qualitative analysis of potentially harmful compounds such as drugs, phthalate-based plasticizers and pesticides were performed directly from the sample surfaces of pills, toys and fruits.

New Aspects

Laboratory-independent and portable DESI-source for in-field measurements, allowing optimized and simplified measurement procedures.

Keywords

Instrumentation, ambient ionization, in-field mass spectrometry, DESI

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2ω-FT-ICR Mass Spectrometry with Quadrupolar Detection

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The advantage of the double-frequency (2ω) detection in FT-ICR over single-frequency (1ω) detection is that it provides twice the resolving power (RP), or allows measurements with 1ω-equivalent RP in half of the time. Multi electrode detections were proposed decades ago but never successfully implemented because of the dominant presence of abundant 1ω-harmonics and weak multi-frequency signals.

Experimenteller Teil

Our techniques to control the magnetron motion in the ICR cell applied to 1ω-detections were also essential to significantly reduce the 1ω-harmonics in 2ω-detections. New detection electronics improve the 2ω signal intensities and allow fast switching between excitation and detection modes using the same electrodes. Furthermore, it allows 1ω as well as 2ω-detections switchable by software-control.

Ergebnisse und Diskussion

The 2ω detection measurements were performed at 7T in a dynamically harmonized cell. Using 2ω-detection in narrowband the 1ω resolving power of 30Mio. at m/z 702 was increased to 60Mio. Oil deposits were studied by applying APPI, ESI and LDI also using absorption mode processing (AMP). RP: 800,000 with 1ω; 1.6Mio. with 2ω; >2Mio. with 2ω+AMP. More than 17,000 molecular formulae were identified in an oil deposit sample with an RMS mass error <150ppb. Over 50,000 molecular formulae could be identified with a similar RMS mass error using continuous accumulation of selected ions (CASI) in a mass window of 55Da. For isotopic fine structure (IFS) in real-time, a mixture of pharmaceuticals was analyzed with LC/MS (duty cycle of 1Hz) leading to a broadband RP of 450,000 at m/z 400. Isotopic patterns reveal IFS with excellent correlation to relative ratios of individual atoms and accurate masses.

Neue Aspekte

Routine 2ω-detection of fundamental resonance frequency doubling the resolving power or reducing the measurement time.

APPI-FAIMS-FTMS source and electrode optimization for the elucidation of structural features of crude oil constituents

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Introduction

The comprehensive analysis of crude oil is one of the most challenging tasks in modern analytics. The main problem in this regard is the unmatched complexity of the sample with reports estimating well over one million distinct compounds present. As a result ultra-high resolving mass spectrometry needs to be used to resolve relevant isobaric species. Additionally, different ionization techniques need to be employed to cover the broad range of polarities of the analytes present within crude oil. Still, one major problem for the mass spectrometric analysis of crude oil is the inability to distinguish isomeric compounds. This issue is addressed by using an ion mobility approach with a lab-build photoionization source and a modified set of FAIMS electrodes.

Experimental

Heavy crude oil was diluted in toluene to a final concentration of 500 ppm and used for analysis by direct injection at a flow rate of 20 µL min^{-1}. Mass spectra were recorded using an Orbitrap Elite, equipped with a FAIMS unit and a lab-built Photoionization source. Selected *m/z* ranges were recorded in SIM mode prior to recording MS/MS spectra after CID at a mass resolving power of 480k (FWHM at *m/z* 400), while scanning through a given range of compensation voltage in steps of 0.2 V. The APPI source was extended by a pusher electrode, held at 1.5 kV. Additional measurements were performed using a modified set of FAIMS-electrodes with a reduced gap of 2.25 cm (standard: 2.5 cm).

Results

Compared to the original source design, an additional pusher electrode was implemented to increase ion transmission into the FAIMS unit. The application of a potential of 1.5 – 2.0 kV resulted in an increase of signal intensity by a factor of 100 – 500 as established using standard compounds of polyaromatic hydrocarbons. The effects of an increased electrical field strength were tested by the implementation of a modified electrode set with a narrower electrode gap. Here, the CV range over which ions of a given composition are distributed is slightly increased. Using Collision Induced Fragmentation in the linear ion trap of the instrument allowed following up on structural features of the transmitted ions. For all monitored ions, generally the loss of fully saturated alkyl chains is dominant throughout the CV range. This is in good agreement with the assumption of polyaromatic (heterocyclic) hydrocarbons with one central aromatic motif that is more or less extensively alkylated. Loss of substituents including aromatic rings are hardly found and generally of low abundance.

New Aspects

The fragmentation behavior of non-polar, isomeric crude oil components was followed by FAIMS-FTMS using MS/MS.

Keywords

FAIMS – FTMS – APPI – isomer separation – crude oil

Titel:

An Integrated Mass Spectrometry Based Approach to Probe the Structure of the Full-Length Wild-Type Tetrameric p53 Tumor Suppressor

Autoren:

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Introduction:

The tetrameric tumor suppressor protein p53 is a transcription factor that binds to specific response-element DNA. P53 plays a crucial role in cancer prevention and is often referred to as the "guardian of the genome". It is one of the most studied and prominent representatives of intrinsically disordered proteins (IDPs). These pose challenges for classical structure elucidation methods, such as X-ray crystallography or NMR spectroscopy. Here, we present an integrated approach for investigating the topology of proteins by combining native mass spectrometry (MS) and cross-linking/MS in one workflow. By this, we obtain structural insights into the p53 tetramer and gain information on the cross-linking efficiency as well as the impact of cross-linker modification on the conformation of an IDP [1].

Words: 120/120

Material/Methods:

^{15}N-labeled and non-labeled p53 were mixed at a molar ratio of 1:1 (10 µM) and pre-incubated in absence and presence of response element DNA. Cross-linking reactions were carried out with 5-fold to 50-fold molar excess of the homobifunctional amine-reactive, MS/MS cleavable cross-linker BuUrBu [2] and 20-fold to 8000-fold molar excess of the heterobifunctional amine-/carboxyl-reactive DMTMM [3] over the p53 monomer. Quenched reaction mixtures were directly used for native MS measurements on a high-mass Q-TOF II instrument (Waters Micromass/MS Vision) or cross-linking/MS analysis, respectively. Cross-linked samples were digested and the resulting peptide mixtures were subjected to nanoHPLC/nano-ESI-MS/MS on an Orbitrap Fusion Tribrid instrument (Thermo Fisher Scientific, San Jose). Cross-links were identified using the in-house software tools MeroX [4] and StavroX [5].

Words: 119/120

Results and Discussion:

P53 contains a high percentage of intrinsically disordered regions, making it inherently difficult to be studied by conventional methods for protein 3D-structure-analysis. Here, we present an integrated approach for deriving structural information of full-length wild-type p53

in solution. To discriminate between intra- (within one p53 monomer) and intermolecular (between two p53 monomers) cross-linked products an isotope labeling approach relying on a mixture of non-labeled (^{14}N) and fully ^{15}N-labeled protein was used. LC/MS/MS-analysis confirmed the cross-linked products based on characteristic mass shifts caused by ^{15}N-labeling and the characteristic doublet signals created during CID-MS/MS fragmentation of the cleavable cross-linker BuUrBu. In conclusion, 14 unique intramolecular and 9 intermolecular cross-links were identified for the p53 tetramer. The cross-links identified in the presence and absence of response element DNA were highly similar, indicating comparable conformations of the *C*-terminal region in the free and DNA-bound p53 tetramer. To determine whether the DNA-binding capabilities of the p53 tetramer are retained after cross-linking; we combined cross-linking with native MS. We performed the cross-linking reactions with varying concentrations of the BuUrBu cross-linker (5-fold to 50-fold molar excess over p53) and conducted native MS measurements directly with these cross-linked samples. Indeed, our MS measurements revealed that DNA binding of the p53 tetramer is retained when using BuUrBu. Nevertheless for DMTMM, the DNA-binding ability of the p53 tetramer is already significantly lowered at a 20-fold molar excess of cross-linker and is completely lost at a 100-fold molar excess of DMTMM. In conclusion, the integration of chemical cross-linking with native MS as complementary techniques is a powerful tool for protein structure elucidation. For the first time, the two techniques were combined in one workflow to obtain not only structural insights into the p53 tetramer, but also to gain information on the impact of cross-linker modification on the conformation of an IDP.

Words 300/300

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Keywords:

p53, MS/MS Cleavable Cross-linker, Stable Isotope Labeling, Native MS

Novel Aspect:

Combine chemical cross-linking and native mass spectrometry in an integrated workflow to investigate an intrinsically disordered protein.

Applications of non-covalently bound membrane proteins in nanodiscs using LILBID-MS

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Introduction:

Particularly challenging to investigate with MS are membrane protein complexes as they require e.g. detergents for solubilization. However some complexes are not stable in detergents. For those, we employ alternative means of solubilisation. Here we focus on nanodiscs (ND) consisting of lipids which more closely mimic the lipid bilayer of the membrane. We used our homebuilt LILBID-MS (Laser-Induced-Liquid-Bead-Ion-Desorption) to answer different biological questions about membrane proteins embedded in ND.

Experimental Part:

A piezo-driven droplet generator is used to produce droplets of 30 µm diameter. The droplets are transferred to high vacuum and irradiated by an IR laser operating at 2.94 µm, a vibrational absorption wavelength of water. This leads to an explosive expansion of the sample droplet. The solvated analyte ions are released and analyzed by a homebuilt reflectron-time-of-flight (TOF) setup [1].

Results and Discussions:

Recently we showed that LILBID-MS is able to reveal the oligomeric state of membrane proteins directly from Nanodiscs (ND) [2].

As an example we present the potassium ion channel KcsA, which is well known to form tetramers. With soft MS conditions in LILBID no dissociation of the KcsA complex occur and we are able to detect the intact KcsA tetramer within the ND. Under harsher laser conditions the complex can be released from the ND, and even dissociated into its subunits, revealing the oligomerization state.

The activity/functionality of many membrane proteins depends on the oligomeric state as we demonstrate for the translocase MraY, which shows a lipid dependent activity. We could show for the first time that MarY is only active as a dimer and the dimer formation is triggered by specific lipids [2]. For the zinc-transporter SV31 we could prove that mutation of the active domain has no influence on the oligomeric state, which we determined to be dimeric [3].

Moreover, LILBID-MS combined with cell-free expression of membrane proteins is able to answer questions about the insertion mechanism of membrane proteins into empty nanodiscs. For instance we could show that this insertion is stepwise and influenced to some parts statistically.

These results confirm that LILBID-MS is a great tool to investigate membrane proteins in ND and is well suited to answer different kinds of biological questions.

New Aspects:

Investigation of membrane proteins in nanodiscs enables to determine the native membrane proteins and enables to answer various biological questions.

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Keywords:

Native mass spectrometry

Nanodiscs

Membrane proteins

Structural characterization of protein-lipid complexes involved in clathrin-mediated endocytosis

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Clathrin-mediated endocytosis is the major trafficking pathway from the plasma membrane to the cytoplasm and thus indispensable for a vast number of cellular processes. Many viruses hijack the host's endocytosis machinery and enter new host cells on this route. Remodeling of membrane curvature during endocytosis requires a mechanical force to be transmitted to the membrane. For this purpose, clathrin adaptor proteins act as linkers between clathrin coat, plasma membrane and actin cytoskeleton. Attachment to the plasma membrane occurs via the membrane associated ANTH and ENTH domains of clathrin adaptor proteins, which were shown to co-assemble in the presence of the phospholipid PI(4,5)P_2. The here presented data on the assembly pathway and the structural characterization of these complexes have implications for a mechanistic understanding of clathrin-mediated endocytosis.

Using native mass spectrometry (MS) we could show that ENTH and ANTH proteins from yeast, fungi and humans possess two PI(4,5)P_2 binding sites and dissociation constants were estimated based on MS binding studies. *H. sapiens* ENTH proteins form a hexameric hub in presence of PI(4,5)P_2. Further oligomerization with ANTH proteins was also found to be PI(4,5)P_2 dependent and mature complexes contain more phospholipids than expected from previous binding studies. Interestingly, we could show that only one subfamily of ANTH domain containing proteins has the capability to form oligomeric complexes with ENTH-domains and results from X-ray crystallography reveal structural differences between the two ANTH subfamilies.

Native MS was used to investigate complex stoichiometries for co-assembled ANTH/ENTH/PI(4,5)P_2-complexes from three different species and gas-phase dissociation of non-covalent complexes gave insights into complex topologies. Formation of chimeric assemblies between the three different species highlights the universal principle of clathrin adaptor protein assembly. Native MS time-course experiments reveal the conversion of smaller complexes, to a larger, more stable form. Taken together, these results, that were confirmed by data from other biophysical techniques (isothermal titration calorimetry, dynamic light scattering, X-ray crystallography) allow us to suggest a complete assembly pathway for the oligomerization of clathrin adaptor proteins.

Steps towards a more native analysis of $Aß_{42}$ using LILBID mass spectrometry

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Alzheimer's disease (AD) is a widespread illness that diminishes the mental skills of patients suffering from it. More than 25 million patients exist worldwide, and the number is predicted to double within the next 20 years [1].

The formation of oligomers of the beta-amyloid peptide (1-42) ($Aß_{42}$) is known to play a key role in AD [2]. The aggregation of $Aß_{42}$ can be analysed with Laser-induced-liquid-bead-ion-desorption (LILBID) mass spectrometry (MS). Usually, the native concentration of $Aß_{42}$ is too low to be studied by MS, thus concentrations higher by orders of magnitude are used for those analysis. We present herein protocols that allow MS analysis of $Aß_{42}$ under more native conditions: lower concentration, higher temperature and using recombinant expressed peptide.

To adapt the sample's properties stepwise towards native conditions we tested the influence of several characteristics on the signal of the MS spectra as well as on the kinetics and the quantity of the forming oligomers. We varied $Aß_{42}$ concentrations, incubation temperatures and tested for differences of synthetic and recombinantly prepared $Aß_{42}$.

To study the oligomerisation we employed LILBID MS. Thereby, a piezo-driven droplet generator produces droplets (50 µm diameter) which are transferred into vacuum and irradiated by IR laser pulses. This leads to release of the analyte-ions into gas phase where they are mass-analysed by time-of-flight.

Using LILBID-MS enables it to quantify the relative amount of $Aß_{42}$ oligomers and thereby to analyse influences of different sample characteristics.

To test the influence of $Aß_{42}$ concentration on MS spectra and on the behaviour of oligomerisation we incubated $Aß_{42}$ at three different concentrations (100, 25, 10 µM). We can show that LILBID-MS allows to detect $Aß_{42}$ oligomers also in a concentration which is lowered by factor of 10 compared to previous results. Reducing the concentration diminishes oligomerisation, but brings a more native-like situation.

Also the temperature should influence the kinetics of $Aß_{42}$ oligomerisation. Therefore, we incubated $Aß_{42}$ at two different temperatures (4°C, 22°C) and checked for the influence of the kinetics of $Aß_{42}$ oligomerisation. As expected, increasing the incubation temperature accelerates the oligomerisation. A temperature shift towards 37°C also brings a more native like situation.

Using synthetically produced $Aß_{42}$ brings some disadvantages. Next to being expensive and less native the reproducibility of the kinetics and the magnitude of oligomerisation is poor. Therefore, Walsh et al. [3] published a procedure to generate recombinant expressed $Aß_{42}$. We adapted this sample

preparation for native MS analysis. We tested both, synthetic and recombinant $Aß_{42}$ to check for differences in MS analysis. Having the same properties, the recombinant protein shows a higher signal-to-noise ratio. The reproducibility of the kinetics and the oligomerisation magnitude is higher than for the case of synthetic $Aß_{42}$.

The most promising settings were used to check the influence of two compounds on the two samples. Using the synthetic $Aß_{42}$ we tested the effect of bexarotene on the oligomerisation, a known decelerator of the oligomerisation. We found that bexarotene influences the primary oligomerisation step and shifts thereby the kinetics about 60 minutes in time. Using the recombinant $Aß_{42}$ we tested the effect of the small molecule BMS493. BMS493 influences two separate steps in the oligomerisation process and thereby shifts the kinetics twice. The overall shift in time is about 100 minutes.

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Polyamine modifications in biosilica-associated proteome

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Diatoms are unicellular algae that produce species-specifically patterned cell walls made from biosilica. Several diatom proteins, termed silaffins, involved in biosilica formation have been characterized [1]. Silaffins are extensively modified and most of their lysine residues bear polyamine chains of varying chemical structures, which are crucial for the proteins' capability to induce silica formation [1]. Species specific patterns of polyamine modifications in silaffins are hypothesized to be required for generating the specific silica morphology [2]. However, to date no information is available on the polyamine patterns in silaffins from different diatom species. Here we report a new analytical approach for comprehensive profiling of polyamine modifications. Remarkably, the resulting data correlate well with the phylogenetic relationships of the analysed diatoms.

Experimenteller Teil

Isolation of diatom biosilica from *Thalassiosira pseudonana*, *T. oceanica*, and *Cyclotella cryptica* was performed as described [3].The mineral component of biosilica was dissolved and proteins solubilised by ammonium fluoride [4] under acidic conditions. The soluble fraction was hydrolysed with 6N HCl at 110°C for 24 hours and hydrolysate was derivatized with AQC (6-aminoquinolyl-N-hydroxysuccinimidyl carbamate) and subjected to LC and quantified by LC-MS on QE Orbitrap (Thermo Scientific). Modifications were mapped back to protein sequences by geLC-MS/MS [5].

Ergebnisse und Diskussion

The whole biosilica-associated protein extracts were subjected to exhaustive acidic hydrolysis and hydrolysates containing lysines modified by polyamine chains were treated with AQC, which quantitatively derivatizes primary and secondary amino groups. Derivatized polyamines were quantified by LC-MS using XIC peaks reconstructed for pre-calculated *m/z* of plausible molecular ions and confirmed by MS/MS. In total 17 polyamine modifications, including 6 novel structures, were discovered. We found that the same pool of polyamine modifications is shared across the three diatom species, however their abundance differ significantly and, in large, reflect the phylogenetic proximity. Interestingly, polyamine-modified hydroxylysine residues contained an acid-resistant phosphoester moiety whose structure was confirmed by ^{31}P-NMR. Fifty one modifications were localized at the protein sequence by retroactive mapping of the expected masses and confirmed by MS/MS.

Neue Aspekte

Comprehensive quantitative profiling of polyamine modification in biosilica-associated proteins

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Following the Unfolding and Dissociation of Calmodulin/Munc13 Complexes by Ion Mobility-Mass Spectrometry

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The calcium-binding protein calmodulin (CaM) is a major regulator in biological processes and interacts with a large variety of targets. Among these are neuronal Munc13 proteins, which form a calcium-sensor/effector complex with CaM that controls short-term synaptic plasticity.[1] Structural elucidation is necessary to provide deeper insights into this complex and the CaM binding motif. The protein CaM itself consists of two Ca^{2+} binding domains, which are connected by a flexible helical linker. Compact and dumbbell-like conformations were observed for apo-CaM, while earlier reported complexes with peptides almost exclusively revealed compact structures.[2,3] Here, we systematically investigate the gas-phase structure of CaM complexes with Munc13 derived peptides using ion mobility-mass spectrometry (IM-MS).

Experimenteller Teil

Different Munc13 isoforms were analyzed including wild type and mutant sequences of a minimal CaM-binding motif as well as elongated peptide sequences. Experiments were performed on a commercially available Synapt G2-S (Waters), in which the traveling wave cell was replaced by a RF-confining drift cell. This modification enables the determination of absolute collision cross sections (CCS) directly from the drift time without external calibration. Protein complex unfolding and dissociation experiments were performed by tandem IM-MS, with the collisional activation being carried out in the ion trap cell prior to the ion mobility drift cell.

Ergebnisse und Diskussion

In the mass spectra narrow charge state distributions are detected for all complexes with a preferred complex stoichiometry of CaM/Peptide/Ca^{2+} 1/1/4, when calcium was added to the sample solution. Ion mobility data, which was investigated in detail for charge state 8, show a defined conformational family for most of the peptide-complexes and the corresponding collision cross section values suggest the compact-canonical type, where CaM is wrapped around the peptide. To get a deeper understanding on the peptide-protein interactions, collision induced unfolding and collision induced dissociation experiments were performed. The resulting data reveal evident differences in dissociation pathways and relative energies. The unfolding pathways are similar for most peptide complexes with a gradual transition from the non-activated compact to a highly-activated extended conformer. However, two CaM-complexes with elongated peptides show an explicit species for medium activation energies. This stable conformation points to a different unfolding pathway for these particular complexes and hints to different binding interactions with these two peptides.

Neue Aspekte

Structural insights in CaM-Munc13 complexes obtained with ion mobility-mass spectrometry

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2-Benzylindane radical cations in the gas phase (I): Substituent effects on a stereoselective McLafferty reaction and related hydrogen transfer processes

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The unimolecular fragmentation of the radical cations of 2-benzylindane and eleven derivatives bearing *meta*- or *para*-substituents at the benzylic moiety has been studied with a special focus on the hydrogen exchange that precedes the McLafferty reaction. Standard EI mass spectra, low-energy (11 eV) mass spectra and mass-analyzed ion kinetic energy (MIKE) spectra were recorded to probe the excitation-energy and ion-lifetime dependence of the fragmentation and the hydrogen exchange. Density-functional theory calculations were used to rationalize the substituent effects on the competition between the benzylic cleavage and the McLafferty reaction and to clarify the role of the distonic arenium ion-type intermediate formed by the γ-hydrogen-transfer step of the McLafferty reaction [1].

Experimenteller Teil

The synthesis of the unlabelled 2-benzylindanes is briefly described. The standard 70 eV mass spectra were recorded with a 311 A double-focusing mass spectrometer (Finnigan MAT, Bremen, Germany) at 3.0 kV accelerating voltage. Other than standard mass spectra (70 eV and 11 eV) as well as the mass-analyzed ion kinetic energy (MIKE) spectra were measured with a ZAB-2F double-focusing instruments (Vacuum Generators, Manchester, UK) at 6.0 kV accelerating voltage and 100 mA trap current. Molecular orbital calculations were performed with the Gaussian 03 suite of programs [2].

Ergebnisse und Diskussion

The experimentally observed substituent effects on the fragmentation of the radical cations of various substituted 2-benzylindanes, as probed for three different energy and ion-lifetime regimes, have been rationalized by means of theoretical calculations of the corresponding enthalpy profiles. The energy requirements for the McLafferty reaction and the benzylic cleavage depend strongly on the position and the electronic nature of the substituent in each case, and the dominance of the McLafferty reaction for the *meta*-substituted isomers agrees with the energetically favorable formation of the distonic ion intermediates formed by the γ-hydrogen transfer step. As will be shown in the accompanying poster, the extent of progression of the 4-H exchange process in the various molecular ions also agrees qualitatively with the depth of the "isomerization valley" relative to the fragmentation threshold [3].

Neue Aspekte

Substituent effects on ion lifetime-dependent competing fragmentation of radical cations.

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2-Benzylindane radical cations in the gas phase (II): Substituenteffects on regio- and stereoselective progressive hydrogen scramblingoccurring prior to unimolecular fragmentation

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In the preceding poster [1], the unimolecular fragmentation of the radical cations of 2-benzylindane and eleven derivatives bearing *meta*- or *para*-substituents at the benzylic moiety has been studied with respect to the hydrogen exchange that precedes their fragmentation by the McLafferty reaction and the energetics and the ions' life-time dependence of the competing fragmentation channels.

Experimenteller Teil

The synthesis of the deuterium-labelled 2-benzylindanes is briefly described. The standard 70 eV mass spectra were recorded with a 311 A double-focusing mass spectrometer (Finnigan MAT, Bremen, Germany) at 3.0 kV accelerating voltage. Other than standard mass spectra (70 eV and 11 eV) as well as the mass-analyzed ion kinetic energy (MIKE) spectra were measured with a ZAB-2F double-focusing instruments (Vacuum Generators, Manchester, UK) at 6.0 kV accelerating voltage and 100 mA trap current.

Ergebnisse und Diskussion

The extensive regio- and stereospecific deuterium labelling experiments confirm that the hydrogen exchange involves the two *cis*-oriented H atoms at the benzylic C-1 and C-3 positions of the indanyl moiety and the two *ortho*-H atoms of the benzyl group. This 4-H exchange is perfectly stereoselective for the most electron-rich congeners [X = OCH_3, $N(CH_3)_2$ and 3',5'-$(OCH_3)_2$] but less stereoselective for the other analogs. Energy- and lifetime-dependent measurements with the deuterium-labelled isotopologs revealed that the extent of H/D exchange progresses with the ions' lifetime much faster in the *meta*- than in the *para*-isomers. With exception of the *meta*-dimethylamino derivative, equilibration (complete scrambling) of the four H atoms is reached in the long-lived, metastable ions, whereas the *para*-dimethylamino isomer does not undergo any exchange at all. The relative rate of the H/D exchange is rationalized on the basis of the energy profiles calculated for the reversible γ-H transfer that generates the corresponding distonic arenium-ion intermediates and for the overall fragmentation by the McLafferty reaction. The *ipso*-protonolysis of the benzyl residue giving rise to the loss of the corresponding arenes specifically from some of the *para*-isomers was also found to reflect the regio- and stereoselective 4-H exchange [2,3].

Neue Aspekte

Substituent effects on the ion lifetime-dependent H/D exchange that precedes the McLafferty reaction of 2-benzylindane radical cations.

Referenzen

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REMPI-Spektroskopie von nicht-kovalenten Anisol-Clustern

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Einleitung

Nicht-kovalente Interaktionen zwischen Molekülen spielen eine Rolle beim Verständnis und der Erklärung von supramolekularen Organisationen und Erkennungsprozessen, z.B. bei DNA Basenpaaren.

Erste Untersuchungen mittels Resonanzverstärkter-Multiphotonen-Ionisation (REMPI) an Benzol- und Phenol-Dimeren zeigen, dass diese eine andere elektronische Struktur aufweisen als die jeweiligen Monomere. Die Spektren weisen jeweils zwei elektronische Grundzustände auf, die bezüglich des Monomers rot- (für den Elektronendonor) bzw. blauverschoben (für den Elektronenakzeptor) sind. [1].

Das REMPI-Spektrum des Anisol-Phenol-Clusters zeigt nur den 0-0-Übergang. Dieser ist rotverschoben zu den jeweiligen Monomer-0-0-Übergängen.

Es wird davon ausgegangen, dass sich eine Wasserstoffbrückenbindung zwischen den Molekülen aufbaut [1].

Die untersuchten Anisol-Cluster verhalten sich anders als Benzole oder Phenole. Vorangegangene Untersuchungen in unserem Arbeitskreis zeigen, dass die Anisol-Cluster einen gemeinsamen elektronischen Grundzustand aufweisen. Dieser ist gegenüber dem Anisol-Dimer rotverschoben ist [2].

Experimenteller Teil

Alle Messungen wurden an einem modifizierten ReTOF-MS durchgeführt. Die Probenzufuhr erfolgte mittels eines gepulsten Molekularstrahls mit Argon als Trägergas (3,5 bar).

Die Probenmoleküle wurden mittels eines durchstimmbaren FL3002 Farbstofflasers (Lambda Physik) ionisiert. Als Pumplaser wurde ein Excimerlaser (Lambda Physik, 308 nm) verwendet [3]. Die verwendeten Laserfarbstoffe waren hierbei Coumarin 307 (250 nm bis 258 nm, frequenzverdoppelt) und Coumarin 153 (258 nm bis 269 nm, frequenzverdoppelt).

Die entstandenen Ionen wurden nach dem Passieren des Reflektors mittels einer *microchannel plate* (MCP) verbunden mit einem LSA1000 Oszilloskop detektiert.

Ergebnisse und Diskussion

Ziel war es die für die Komplexierungspartner Toluol, Xylol, Mesitylen, Phenetol, Kresol und Xylenol erhaltenen Ergebnisse an einem anderen experimentellen Aufbau zu reproduzieren [2,3]. Dieser wurde hierfür derart modifiziert, dass die Erzeugung der Ionen statt mit Elektronenionisation mittels REMPI erfolgen kann.

Ergänzend zur Anwendung des Messprinzips an einem neuen Aufbau wurden die Fragmente der Cluster näher untersucht und leistungsabhängige Messungen durchgeführt. Zusätzlich

wurden metastabile Ionen betrachtet, um die Fragmentierungspfade der Cluster näher zu untersuchen.
Anschließend sollen die Untersuchungen mit anderen Komplexierungspartnern fortgeführt werden. Somit sollen die aus früheren Arbeiten erhaltenen Ergebnisse an weiteren substituierten Benzol-Derivaten überprüft und der Einfluss auf die elektronische Struktur der Cluster untersucht werden. Zusätzlich soll das Modellsystem schrittweise erweitert werden, um es den tatsächlichen chemischen Eigenschaften der DNA weiter anzunähern.

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Neue Aspekte

REMPI-Spektren neuer Anisol-Cluster, Untersuchungen metastabiler Cluster-Ionen.

Stichworte

REMPI
Flugzeitmassenspektrometrie
Cluster

Resolution enhancement by delayed ion extraction in a single-particle aerosol mass spectrometer

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Keywords: mass spectrometry, fullerenes, instrumentation, single particle analysis

Introduction

Compensation of initial ion energy spreads by delayed ion extraction in a time-of-flight mass analyzer is a widely used technique to improve mass resolution within a limited mass range [1]. For single-particle aerosol mass spectrometers this method is not very common. In our study we incorporated a delay generator into the 'LAMPAS 3' aerosol mass spectrometer. By using delay times between ionization event and ion extraction of 285 to 685 ns, an optimum was found for a delay of 285 ns. With 2.95 kV total extraction voltage the mass resolution for positively charged fullerene ions (m/z = 720 u) was improved by a factor of 1.7 compared to direct ion extraction.

Method

The compact mobile reflector laser mass spectrometer LAMPAS 3 (19" rack, 150 cm in height) is used for the simultaneous detection of positively and negatively charged ions from single aerosol particles. For this initial study, ion extraction voltages of 3.55 and 2.95 kV for negative and positive ions were used. A delay generator (DG535, Stanford Research Systems, Sunnyvale CA, USA) was integrated into the existing electronics and triggered by the 337 nm nitrogen laser. The minimum delay was 285 ns, limited by the time delays of delay generator, high voltage switch and nitrogen laser. The upper mass limit of m/z = 300 was extended to m/z = 1000 in order to detect ions generated from fullerene particles at 720 u.

Results

For both ion polarities mass resolution (fwhm) of fullerene ions was determined by direct extraction of ions and was compared to mass resolution of respective ions after delayed ion extraction. The delay time was varied between 285 and 685 ns. For positively charged C_{58} ions an optimum delay time of 285 ns was found to increase mass resolution $m/\Delta m$ (fwhm) from 161 to 268. For negatively charged ions a smaller increase was observed. Compared to desorption methods such as MALDI, where the direction of the ion plume is well-defined,

the enhancement in mass resolution is stronger for ions formed from single particles homogeneously into all directions. An additional effect was observed for the fragmentation of fullerene ions, expressing a shift to higher-mass fragment ions with longer delay times. The unfragmented C^+_{60} ion was predominately seen after longer delay times, while intensities of smaller fragment ions (C^+_{58}, C^+_{56}, C^+_{54}, …) decreased. This can be explained by the lower internal energy of the C_{60} ions after evaporative and collisional cooling of the plume prior to ion acceleration, but may also be caused by the lower density of colliding ions and neutrals at the acceleration event [2]. The sensitivity of the system was increased with respect to less fragmented ion species, allowing for an easier interpretation of mass spectra of larger organic molecules. The new instrumental design of the LAMPAS 3 mass spectrometer led to an extended mass range and increased mass resolution.

Acknowledgement

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Novelty

A mass resolution enhancement by delayed ion extraction was achieved for simultaneous detection of positively and negatively charged ions from single particles.

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Aggregation of a crown-ether decorated zinc-phthalocyanine by collision-induced desolvation providing insight into the electrospray mechanism

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Einleitung

The aggregation of phthalocyanines (**Pc**s) is well known in solution and depends on both the concentration and the choice of solvent [1]. Pcs preferentially stack with a small staggering angle to optimise the π-π interactions between the molecules [2, 3]. Crown-ether decorated Pcs were initially synthesised to create more well-defined structures. The addition of metal ions results in the formation of rigidly eclipsed dimers and oligomers in which the cations are sandwiched between the crown ethers [1, 4].

Though the aggregation in solution has been studied extensively, it has never been examined in the gas phase. We investigated the tetra-[18]crown-6 ether functionalized zinc-phthalocyanine (ZnPcTetCr, **M**) with electrospray ionization mass spectrometry (ESI-MS) in the absence of coordinating metal cations [5].

Experimenteller Teil

ZnPcTetCr was dissolved in dichloromethane (DCM) and then diluted with toluene (Tol) (4:1, v:v) to give a final concentration of 1-5 × 10^{-5} mol L^{-1} . The solvents were chosen to avoid protonation and sodiation of the crown ether moieties. The ESI-MS experiments were performed with three different mass spectrometers, a quadrupole ion trap (Esquire6000, Bruker Daltonics, Germany) and two quadrupole time-of-flight instruments with high (micrOTOF QII, Bruker) and ultra-high resolution (maXis 4G, Bruker).

Ergebnisse und Diskussion

When sprayed from aprotic, sodium-free solvents, ZnPcTetCr can be observed as a radical cation $\mathbf{M}^{+\bullet}$. In addition, various singly and multiply charged aggregates of the form $\mathbf{M}_n^{z(+\bullet)}$ were observed. These are bound together only by electrostatic interactions, without alkali metal cations inside the crown ethers.

Collision-induced dissociation (CID) experiments indicate that these clusters consist of stacked neutral **M** and radical cations $\mathbf{M}^{+\bullet}$. The aggregates are probably stabilised by charge transfer between adjacent molecules.

While the radical ions $\mathbf{M^{+\bullet}}$ are generated by electrochemical oxidation of individual molecules in the spray needle, the aggregation of charged and neutral molecules is proposed to occur during the desolvation process. When the solvent evaporates from the charged droplets, the concentration of the Pcs increases and they form stacks. Complete evaporation of the solvent and detection of the aggregates was found to require an additional acceleration of the droplets in the transfer region of the instrument (dual ion funnel), the resulting collisions with neutral gas assisting the desolvation process.

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Neue Aspekte

The aggregation of crown-ether decorated phthalocyanines in the absence of metal cations was first demonstrated in the gas phase.

Stichworte: electrospray, phthalocyanine, crown ether, cluster, aggregate

Thema: Gasphasenreaktionen & Fragmentierungen; Ionisationsmethoden

Kategorie: phthalocyanine, cluster

Direct Observation and Reactivity Studies of Organoferrates by Electrospray Ionization Mass Spectrometry

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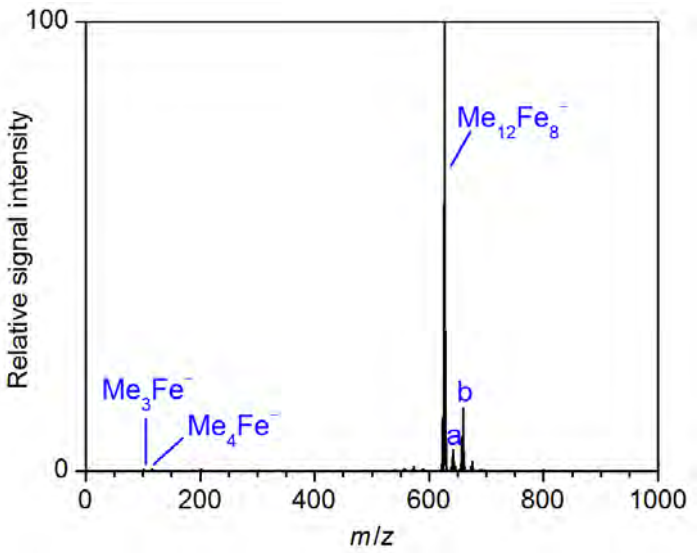

Figure: Resulting negative ion-mode ESI mass spectrum of the products formed in the reaction of $Fe(acac)_3$ with 4 eq. MeMgBr in THF; a = $Me_{13}Fe_8^-$, b = $[Me_{12},Fe_8,O_2]^-$.

Iron-catalyzed cross coupling reactions have a great potential thanks to the easy accessibility, low cost and non-toxicity of iron-catalysts, but the insufficient mechanistic understanding restricts their application.[1,2] The nature of the in situ formed intermediates is discussed controversially with iron in oxidation states ranging from -II to +III. Notwithstanding this ambiguity, growing evidence points to the prominent role of negatively charged organoiron complexes in iron-catalyzed cross-coupling reactions.[3]

An ideal method to analyze such in situ formed organoferrates is electrospray-ionization mass spectrometry (ESI-MS).[4,5] Additional gas-phase fragmentation experiments and kinetic measurements help to probe their individual reactivity in solution and in the gas-phase.

Sample solutions (prepared under inert atmosphere in tetrahydrofuran) were subjected into the ESI source of a HCT quadrupole ion trap from Bruker Daltonik with a motor-driven gas-tight syringe. The ESI source was operated under mild conditions (333 K) to prevent labile organometallic species from unwanted decomposition reactions. Observed ions were identified on basis of their *m*/*z* ratio, their isotope pattern and their behavior in the gas-phase.

Fragmentation experiments of mass-selected ions were performed in a helium-filled ion trap via collision-induced dissociation (CID). For monitoring the evolution of the ESI signal intensities in time, mass spectra were recorded with alternating ion polarity and averaging of 50 *m*/*z* scans.

For further mechanistic insight we analyzed sample solution of Fe(III) with PhMgCl (4 eq.) in tetrahydrofuran (THF) via ESI mass spectrometry.[4] Dependent on the presence of common additives or ligands different homoleptic mononuclear and polynuclear anionic organoiron complexes could be observed with iron in oxidation states ranging from Fe(-I) to Fe(III). Addition of electrophilic substrates like ^{i}PrCl resulted in the formation of intermediates, such as $Ph_3Fe^{i}Pr^{-}$, which undergoes reductive elimination of the cross-coupling product in gas-phase experiment offering the possibility to observe directly the putative key elementary step of iron-catalyzed cross-coupling reaction. We monitored the time profiles of the ESI signal intensities of the anions present in the reaction of in situ formed phenylferrates with ^{i}PrCl showing that $Ph_3Fe^{i}Pr^{-}$ is formed via the homoleptic iron(II) complex Ph_3Fe^{-} (or by organoiron species being in fast equilibrium with this complex).

The resulting negative ion-mode ESI mass spectrum of a reaction solution of Fe(III) with MeMgCl (4 eq.) in THF was dominated by the octanuclear cluster anion $Me_{12}Fe_8^{-}$ (figure).[5] With a combination of ESI mass spectrometry, deuteration experiments and gas-phase fragmentation experiments it was possible to learn more about its behavior in solution and in the gas-phase. The air- and moisture-sensitive $Me_{12}Fe_8^{-}$ as well as its deuterated analogue $(CD_3)_{12}Fe_8^{-}$ showed a diverse unimolecular reactivity. Beside the loss of methyl radicals, the elimination of dimethyliron, dihydrogen and methane could be observed resulting in the putative formation of iron-carbene units in the gas-phase. With the aim to make neutral organoiron intermediates visible we added cationic charged-tags as electrophilic substrates to in situ formed methylferrates. We could observe the cross-coupling product in the resulting positive ion-mode ESI mass spectrum, but the absence of any iron-containing cations points to the short lifetime of such reaction intermediates.

In summary the identification of organoferrates and their reactivity in solution and in the gas-phase improved our mechanistic understanding of iron-catalyzed cross-coupling reactions.

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Improving the sequence coverage in top-down MS/MS of proteins

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Einleitung: A major issue in top down proteomics is to achieve high sequence coverage to unambiguously identify and characterize (e.g. posttranslational modifications) the target protein. Several parameters are known to influence the MS/MS efficiency, such as the ion activation mechanism (CID, HCD and ETD), the collision energy applied and the charge state of the precursor ion. The aim of the present study was to elucidate the effect of using supercharging reagents on the MS/MS efficiency in ESI MS/MS experiments with a model protein, Cytochrome C. Secondly, the influence of the ion activation energies in HCD experiment on the generation of ion series was studied.

Experimenteller Teil: Cytochrome C (*Equus caballus*) in its mature form (104 amino acids, N-terminus acetylated, Heme C covalently bound to Cys-14 and Cys-17, 12.36 kDa) was diluted in 0.1 % FA/50 % ACN to a concentration of 1 pmol/µL and injected offline into a Q Exactive mass spectrometer (Thermo Fisher Scientific) using a heated electrospray source (hESI). The supercharging agents sulfolane and m-nitrobenzyl alcohol (m-NBA) were added at a concentration of 0.1 % (v/v). Precursors of different charge states were manually selected (isolation width 5 m/z) and subjected to higher-energy collisional dissociation (HCD) covering normalized collision energies (NCE) between 12 and 24 % with increments of two percent. The obtained spectra were semi-manually annotated using mMass.

Ergebnisse und Diskussionen: When Cytochrome C was ionized without the addition of supercharging agents, charge states between +9 and +21 were observed with +17 being the most intense precursor. Distributing intensities over thirteen different signals led to overall lower intensities compared to peptides where charge states typically range between +2 and +4. The addition of supercharging agents increased the average charge state and almost doubled the intensity of the most intense signal. Furthermore, the intensities were not distributed as much. The sequence coverages for the most intense precursors, namely +17 for the control and +20 for the sulfolane and m-NBA-assisted samples, at a NCE of 14 were compared. Best results were obtained for the m-NBA-assisted ionization (57 %). The coverage for the sulfolane sample (48 %) was still greater than for the control (36 %). However, this benefit could not be observed at higher NCE values. Interestingly, different fragments were observed at different NCE values hinting at a NCE dependent breakage of peptide bonds in the tested activation energy range. Combining all detected fragments for the sulfolane-assisted ionization between 12 and 24 NCE achieved a sequence coverage of 85 %. This strategy outperformed any single NCE value; the highest sequence coverage of 71 % was achieved for an NCE of 20 %.

The results show that supercharging proteins can enhance the precursor ion intensities, consequently increasing fragment ions' intensities and overall sequence coverage achievable at lower NCE values. The data suggest that for top-down analysis proteins should be fragmented at various activation energies to maximize the overall sequence coverage. These finding are presently being validated by testing proteins of different sizes and physio-chemical properties.

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Stichworte: Proteomics, Top-Down, Intact Protein, Electrospray Ionization, Collision-Induced Dissociation

Constitution and gas phase reactivity of organocobaltates

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Transition metal-catalyzed cross-coupling reactions play a commanding role for carbon-carbon bond formation reactions in organic synthesis.[1] In the last decade cobalt containing catalysts have received particular interest. In comparison to conventional cross-coupling catalysts based on nickel or palladium, the homogenous cobalt catalysis allows an easier formation of sp^3-sp^3 bonds.[2,3] Little is known about the mechanistic details of the cobalt-catalyzed cross-coupling reactions. Because there are proposals involving anionic species, we used electrospray ionization mass spectrometry to detect the in situ formation of cobaltate species.[3] Collision induced dissociation experiments helped to reveal the gas phase reactivity of isolated organocobalt compounds. The samples were prepared under inert atmosphere (argon) at low temperature in tetrahydrofuran and injected into the ESI source of an HCT quadrupole ion trap mass spectrometer from *Bruker Daltonics* using a motor driven gastight syringe. Mild conditions (T = 60 °C) were used to avoid the decomposition of unstable organocobalt species.

Under the chosen conditions it is possible to detect various air- and moisture-sensitive organocobaltate species by ESI mass spectrometry with oxidation states ranging from Co(+I) to Co(+III). The nature of the in situ formed organocobalt complexes, their aggregation and oxidation states strongly depend on the metal of the transmetallation reagent (Mg vs. Li). For example, the transmetallation of Co(II) salt with PhMgCl results in the predominant formation of $MgCo_3Ph_6^-$ whereas the corresponding reaction with PhLi leads to a multitude of cobaltates like $CoPh_4^-$, $Co_3Ph_6^-$ and $Li_2Co_2Ph_5^-$. For some reactions the detection of Mg-containing as well as Li-containing heterobimetallic organocobaltates $M_xCo_yR_z^-$ (M = Mg, Li; R = organic residue) was possible. The temperature of the sample preparation showed a strong influence on the spectra in that lower temperatures permitted the observation of unstable cobaltates. Addition of commonly used ligands, such as isoprene or triphenylphosphane stabilized low oxidation states. For the homoleptic ate-complexes different unimolecular reactivities and dissociation pathways occurred in collision induced dissociation experiments. For the Co(+III) species $CoPh_4^-$, the loss of the homo-coupling product led to Co(+I) complex $CoPh_2^-$. Thus, the reductive elimination as key step of a carbon-carbon bond formation reaction could be monitored directly. Cobaltates with other organic residues showed alternative reaction channels like the loss of radicals $R^\bullet$ or fragments R+H (R = organic residue). Addition of 1-bromobutane to a solution of Co(II) salt and benzyl Grignard formed the heteroleptic ate-complex $BuCoBn_3^-$, which undergoes cross-coupling reaction in gasphase studies.

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Implementation of Ultraviolet Photodissociation on a LTQ FT Ultra Mass Spectrometer and first Applications

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Keywords: Instrumentation, tandem mass spectrometry, UVPD, charge dependence, nESI

Introduction (120)

Tandem mass spectrometry (MS) is a versatile tool to investigate the chemical composition and structural features of molecular ions. Most regularly, tandem MS is performed by colliding ions of selected *m*/*z* ratio with inert gas atoms/molecules causing ion fragmentation and generating diagnostic fragments. Whereas this process known as collision-induced dissociation (CID)[1] finds widespread use in proteomics, metabolomics/lipidomics and organic MS,[2,3] its use for full structural characterization of ions is hampered by the thermochemically/kinetically controlled formation of most fragment ions. In contrast, fragments formed by ultraviolet photodissociation (UVPD) have been shown to originate from specific functional groups and chromophores.[4,5] Therefore, we implemented UVPD on an ion cyclotron resonance mass spectrometer and present first results for small model systems.

Method (120)

All experiments were performed with a 7 T Fourier-transform ion cyclotron resonance (FT-ICR) mass spectrometer (LTQ FT Ultra, Thermo Fisher Scientific GmbH) equipped with an infrared multiphoton dissociation (IRMPD) extension. The IRMPD laser housing was removed and the installed ZnSe window was replaced by a CF flange containing a fused silica window (Hositrad Vacuum Technology). Laser light of a frequency quadrupled (266 nm; Brilliant B, Quantel Laser) and quintupled (213 nm; Tempest, New Wave Research) Nd:YAG laser system was guided into the trapping cell of the FT-ICR mass spectrometer by means of dichroic mirrors, respectively. Positive ions were generated with a nano electrospray ionization (nESI) source employing gold coated offline emitters with 5 µm inner tip diameter (DNU-MS).

Results (300)

A LTQ FT Ultra mass spectrometer was modified to allow for UV light to enter the ICR trap of the instrument and perform UVPD experiments. Two Nd:YAG laser systems generating light of 266 nm and 213 nm at 20 Hz repetition rate with 7 ns pulse length were installed in order to perform UVPD experiments. The timing of the laser pulses was synchronized with the mass spectrometer by means of a home-built delay generator and was connected to the IRMPD synchronization module of the instrument. Dichroic mirrors, aperture systems and lenses were used to guide the UV laser light into the ion trap, define the beam profile and assure an optimal ion cloud-laser light overlap. The UV photofragment yield of [3-iodo-L-tyrosine+H]$^+$ was studied as a function of laser energy, laser beam diameter and number of laser pulses/irradiation time in order to optimize the newly installed UVPD setup. As expected, the dominating fragmentation channel was iodine atom loss when using UV light of 266 nm, whereas CID experiments of [3-iodo-L-tyrosine+H]$^+$ gave rise to the loss of neutral ammonia and formic acid. After optimization, a photofragment yield of ~0.7 was obtained for [3-iodo-L-tyrosine+H]$^+$ hinting to a good overlap of ion cloud and laser light. Additionally, small organic model systems including iodine- and nitrogen-rich compounds and their UV fragmentation were studied as a function of charge carrier (H^+, Na^+, K^+,…), where possible as a function of charge state (+1,+2), and results were compared to corresponding CID mass spectra. For most ions the relative abundance of the fragments or the fragment identity differed between UVPD and CID. Whereas CID fragmentation patterns were dominated by fragments stemming from weakly bound functionalities and leaving groups, UVPD fragments predominately originated from regions of the ion that are in close proximity to the excited chromophore.

Acknowledgement

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New Aspects (20)

Implementation of a dual-color UVPD setup on a LTQ FT Ultra instrument with photofragment yields of ~0.7.

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The internal energy in a MALDI plume probed with thermometer molecules: Effects of laser excitation wavelength and laser fluence

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Derivatives of benzylpyridinium salts are frequently used to gauge the internal energy in desorption/ionization processes [1]. Upon thermal activation, these "thermometer molecules" (TM) fragment predominantly along a certain bond exhibiting a well-defined bond energy. TMs have also been used to probe the matrix-dependent average internal energy of analytes within a MALDI event [2]. In line with general experience, internal energy was found to generally increase with the applied laser fluence. Together with the matrix absorption profile, the excitation laser wavelength constitutes another key factor in MALDI [3]. Using an optical-parametric oscillator (OPO) laser, 2,5-dihydroxybenzoic acid (DHB) as MALDI matrix, and *p*-methoxy-benzylpyridinium chloride as TM, we here probed the mean internal energy in dependence of laser wavelength and laser fluence.

Experimenteller Teil

p-Methoxy-benzylpyridinium chloride was mixed with DHB matrix in a 1:2000 molar ratio. The dried-droplet method was used for preparation of co-crystallized samples on stainless steel plates. In the present MS experiments the wavelength-tunable OPO laser (versaScan, GWU-Lasertechnik) was scanned between 240-340 nm. MALDI-MS measurements were performed with an axial time-of-flight mass spectrometer (4800 TOF/TOF, AB Sciex) in reflector mode (pressure in the ion source, $7x10^{-7}$ mbar, ion extraction voltage, 20 kV, delayed extraction time, 300 ns) and a prototype orthogonal-extracting (oTOF) mass spectrometer [4]. The oTOF was equipped with a modified oMALDI2 ion source, providing variable N_2 buffer gas pressure and low field extraction conditions. Focal spot sizes of the coupled laser beam were ~300x350 μm^2 in both cases.

Ergebnisse und Diskussion

To enable operation of the AB4800 mass spectrometer with the OPO system, various modifications of the trigger electronics and laser beam path were successfully applied. Overall the experiments with this analyzer produced consistent and clear results: In line with the foregoing studies [2], an increase of the laser fluence resulted in a reduction of the survival yield (SY) of the TMs for all probed wavelengths.

To study the effect of the laser wavelength on the SY, the wavelength dependence of the matrix absorptivity had to be considered. By transforming the laser fluence to the mean excitation energy per volume at the sample surface, this effect was deconvoluted to unveil the influence of the wavelength on energy uptake by the TM. At a constant volume energy, SY was lower near 340 nm than at smaller wavelengths. This points to an increased transfer of energy to the TMs with increasing laser wavelength. Generally, sizable fragmentation set in for calculated mean internal energies between 3.0 and 3.6 eV. These findings stand in contrast to our previous wavelength study in which peptide fragmentation increased at lower wavelength and suggest a different energy transfer mechanism [3].

Due the additional collisional cooling and residence time effects, the results obtained with the oTOF analyzer were more difficult, if not impossible, to interpret. In this case, the SY not only depended on the laser irradiation parameters but strongly also on the ion extraction voltage and the buffer gas pressure. This behavior can presumably be interpreted as a superposition of two competing effects, a “cooling-effect” and a “velocity-effect”.

The combined results provide exciting insight into the MALDI mechanisms. Experiments will soon be complemented by including further matrix systems such as cinnamic acid derivatives.

Neue Aspekte

Combined wavelength/fluence study on the internal energies in a MALDI plume as probed with thermometer molecules and axial-/o-TOF mass spectrometers

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Colorful MALDI: Effect of the Laser Excitation Wavelength on the Analytical Sensitivity in Standard MALDI-MS and Imaging Experiments

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MALDI mass spectrometers are typically equipped with either N_2 (337 nm) or Nd:YAG/Nd:YLF lasers (355/349 nm). However, their emission lines are not necessarily matching the absorption bands of some powerful MALDI matrices. At the same time, several studies have shown that an optimal UV-MALDI performance is only obtained if the laser wavelength coincides with a high optical absorptivity [1,2]. Here we compared the performance characteristics of selected MALDI matrices at 337 nm and at individually optimized laser wavelengths. We investigated a set of analyte systems including standard peptides, BSA digest and phospholipids, and determined limits of detection. Imaging experiments were carried out with mouse brain sections. For all studied systems best results were generally obtained after wavelength adjustment.

Experimenteller Teil

Solid state absorption profiles of the MALDI matrices were determined in diffusive reflection geometry using an integrating sphere (SR-260, Shimadzu) and a dual beam spectrophotometer (UV-2102PC, Shimadzu). MS experiments were conducted with a modified Synapt G2-S mass spectrometer (Waters). A wavelength-tunable (213-2550 nm) optical-parametric oscillator (OPO) laser with 5 ns pulse duration (GWU Lasertechnik) served for desorption/ionization. The focal spot size of the laser beam was adjusted to a focal spot of ~10 µm x 20 µm at each wavelength using telescope optics. Pulse energies were individually optimized for each matrix/wavelength system. To determine limits of detections (LODs) dilution series were investigated using the dried-droplet method. Mouse brain sections were coated using sublimation/recrystallization protocols that were optimized for each matrix.

Ergebnisse und Diskussion

For the experiments the following matrix substances were investigated (wavelengths of peak absorption in the solid state are given in parentheses): α-cyano-2,4-difluorocinnamic acid (305 nm), α-cyano-2,3,4,5,6-pentafluorocinnamic acid (295 nm), α-cyano-4-chlorocinnamic acid (310 nm), 5-chloro-2-mercaptobenzothiazole (320 nm), 2,5-dihydroxyacetophenone (370 nm), 2-(4'-hydroxybenzeneazo)benzoic acid (520nm).

Consistently, lower LODs (as compared to 337 nm) were obtained in the standard MALDI-MS experiments when the OPO laser emission was adjusted to the optimal wavelengths of the individual matrices. For example, for the α-cyano-4-chlorocinnamic acid/peptides and 2-(4'-hydroxybenzeneazo)benzoic acid/phospholipids systems, improvements in analytical sensitivity by 2 to 3 orders of magnitude were achieved, providing an LOD in the lower attomole range.

To investigate the wavelength effect in MALDI-MS imaging experiments, one half of coronal mouse brain sections were measured at optimal wavelength and the other half at 337 nm. Generally, the same differences in performance characteristics as found for the standard

MALDI-MS experiments was also obtained in these MALDI-MSI runs. This demonstrates the enormous potential an adjustment of the excitation wavelength can potentially have for imaging applications in which a particular high sensitivity for a certain analyte class is often paramount. Notably, when using the optimal wavelengths, in some cases also less sodium-adducts were detected in favor of an increase in protonated lipid species. In some cases this is an advantage in terms of structure elucidation, enabling tandem MS experiments of the more stable protonated ions.

Neue Aspekte

First study highlighting the relevance of the laser excitation wavelength for particular sensitive MALDI-MS imaging measurements.

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Untersuchung von Limonen-Clustern im LTP-Twin-Trap Massenspektrometer

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Einleitung

Kleine organische Moleküle, vor allem aromatische, neigen unter entsprechenden Bedingungen dazu Cluster zu formen. In der Massenspektrometrie werden solche Komplexe meist durch Photoionisationsverfahren generiert. Im Rahmen dieser Arbeit wurde eine Niedertemperaturplasmaquelle (LTP) für ein Twin-Trap Massenspektrometer konstruiert. Mittels LTP können unpolare bis polare Verbindungen geringer Molekülmasse ionisiert und deren Cluster anschließend untersucht werden. Es zeigte sich, dass unter Atmosphärenbedingungen auch nicht aromatische Verbindungen zu einer Clusterbildung neigen. Als Testsystem wurde (S)-(-)-Limonen gewählt. Mit Hilfe des Twin-Trap Systems können Rückschlüsse auf die Clusterstabilität geschlossen werden.

Experimenteller Teil

Alle Messungen wurden mit einem Twin-Trap Massenspektrometer der Firma *Bruker Daltonik* durchgeführt. Hierbei handelte es sich um einen Prototypen bestehend aus einer Paul-Falle und einer Cassini-Falle entsprechend dem von C. Köster 2015 veröffentlichtem Design [1]. Die Probenzufuhr erfolgte über die Gasphase in das LTP. Als LTP-Quelle ist ein Eigenbau nach dem Design von Nørgaard et al. [2] verwendet worden. Als Plasmagas wurde Argon (99.999 %) verwendet. Nach der Ionisation unter Atmosphärenbedingungen wurden die Ionen in die Paul-Falle überführt. Die Messdaten der Paul-Falle konnten direkt ausgelesen werden. Alternativ konnten die Ionen gespeichert werden und anschließend in die Cassini-Falle weitergeleitet werden. Kalibriert wurden die Massenspektren extern mittels des Low Concentration TuneMix von *Agilent Technologies* unter Verwendung einer Elektrospray-Quelle.

Ergebnisse und Diskussion

Die durchgeführten Untersuchungen zeigten die Bildung verschiedener Cluster des Limonens. Für eine sicherere Zuordnung wurden alle Messungen mit Messungen an einem FT-ICR Massenspektrometer verglichen. Es wurden Cluster bestehend aus mehreren Limonenmolekülen nachgewiesen. Ebenso sind verschiedenste Variationen an oxidierten Spezies vorhanden. Grund hierfür ist, dass die Ionisation unter Atmosphärenbedingungen in Gegenwart von Luft durchgeführt worden ist. Die Spektren, die mit der Paul-Falle aufgezeichnet worden sind, zeigen die stärksten Signale für Cluster der theoretischen Zusammensetzung $[2M+H]^+$, $[2M-2H+H]^+$ und $[2M-4H+H]^+$. Von allen drei Spezies sind die einfach und zweifach oxidierte Form zu finden. Außerdem finden sich Cluster aus Fragmenten einzelner Moleküle. Es wurden Cluster bis zu einer Zusammensetzung aus bis zu vier Limonenmolekülen gefunden. Das in den Spektren der Paul-Falle am stärksten auftretende Signal ist unter den verwendeten Einstellungen das Signal des $[2M-4H+H]^+$. Werden die Ionen nun für eine Zeit von 0,5 bis 200 ms in der Paul-Falle gespeichert und in die Cassini-Falle übergeben so ist die Zahl der Signale stark reduziert. Das prägnanteste Signal ist das Signal des $[2M-2H+H]^+$. Die in der Paul-Falle häufigste Spezies ist folglich nicht die stabilste. Es überdauern demnach nur die stabilsten Cluster die Speicherzeit in der Paul-Falle. Grund hierfür ist vermutlich das Helium, das als Puffergas in der Paul-Falle eingesetzt wird.

Neue Aspekte

Untersuchung von LTP Clusterprozessen organischer Moleküle mittels eines Twin-Trap Massenspektrometers.

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Stichworte

Atmosphärenbedingungen, Cluster, LTP, Twin-Trap, Cassini-Falle

An improved approach for calculating dissociation rates of benzylpyridinium ions

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Introduction: For assessing the limitations of a mass spectrometric method, knowledge of the energy, which is transferred to analytes during the ionization process, is crucial. With respect to electrospray ionzation, the energy conditions were extensively investigated by monitoring survival yields of thermolabile benzylpyridinium ions.[1] For deriving quantitative results from the experimental data, reaction energies and kinetic shifts for the dissociation of the employed benzylpyridinium ions are needed and have to be determined by theory. As the commonly used method for obtaining kinetic shifts for the dissociation of benzylpyridinium ions[2,3] lacks a firm theoretical basis, a more profound approach, namely the Simplified Statistical Adiabatic Channel Model (SSACM),[4,5] was applied in this study.

Methods: B3LYP-D3/cc-pVTZ geometry optimizations were conducted for obtaining the molecular structures for the dissociation of the investigated compounds (*n*-butylbenzene radical cation, *p*-X-benzylpyridinium ions with X = H, Me, OMe, F, Cl, I, NO_2, CF_3, CN). In order to determine accurate zero-point dissociation energies, electronic single point energies were obtained for all final geometries by means of local coupled cluster methods in combination with a cc-pVTZ/cc-pVQZ complete basis set extrapolation. On the basis of the results from the present quantum chemical calculations, microcanonical dissociation rate constants were calculated within the SSACM approach and with the software MassKinetics, which employs RRKM theory. With respect to the SSACM calculations for the dissociation of benzylpyridinium ions, the ion-dipole approximation was applied.

Results and Discussion: The calculated zero-point dissociation energies E_0 of the investigated benzylpyridinium ions are conservatively estimated to have an error of 0.1 eV and, thus, are expected to be the most reliable to date. These E_0 values deviate significantly from the results of previous calculations.
For the dissociation of the *n*-butylbenzene radical cation, which was considered as a benchmark reaction, SSACM calculations according to Troe *et al.*[4] yielded an excellent agreement between theoretical and experimental dissociation rate constants. In contrast, MassKinetics calculations with the typically used input parameters lead to substantial deviations. Based on the results for the dissociaton of the *n*-butylbenzene radical cation, SSACM calculations were conducted for the simple bond fission of the investigated benzylpyridinium ions. Here, the number of activated complex states had to be calculated ab initio. Given the large dipole moment of pyridine, these calculations were done by assuming that the interaction potential of the fragments can be approximated by an ion-dipole interaction. Again, for the dissociation of benzylpyridinium ions, MassKinetics calculations with the commonly applied input parameters resulted in significant deviations from the SSACM results. The MassKinetics calculations predict kinetic shifts for the dissociation of benzylpyridinium ions in a typical quadrupole mass spectrometer, which exceed those derived from the SSACM method by 1 to 2 eV. Although the error of the kinetic shifts derived from the ion-dipole SSACM calculations is difficult to estimate, this approach affords a significant improvement in comparison to the commonly performed RRKM calculations with MassKinetics.

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Keywords: thermometer ions, dissociation energy, kinetic shift, SSACM

Stability and Unimolecular Reactivity of Organopalladate(II) Complexes[1]

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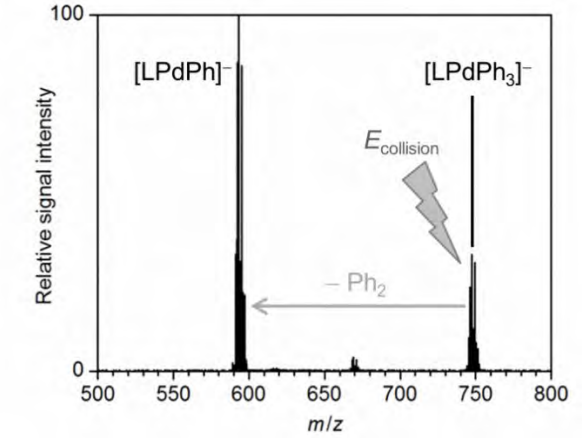

Palladium catalyzed reactions, such as cross-coupling and Heck-type reactions, are widely used in organic synthesis. In many of these transformations, the catalytically active Pd^0 species is obtained by an *in situ*-reduction of a Pd^{II} precursor in the presence of a phosphine ligand (L). This can either be achieved by the phosphine[2] or, possibly, by the stoichiometric organometallic reagent. To investigate the mechanism of the latter reduction pathway, we studied palladate(II) complexes of the type $[L_nPdR_3]^-$ (R = Ph, Bn, Bu; n = 0,1) by Electrospray-Ionization Mass Spectrometry (ESI-MS) and Collision-Induced Dissociation (CID) experiments. Samples were prepared under standard Schlenk conditions by treating solutions of $Pd(OAc)_2$ and 2 equiv. of the phosphine ligand in tetrahydrofuran (THF) with 5 equiv. of the organometallic reagent. ESI-mass spectrometric experiments were carried out with a micrOTOF-Q II instrument (Bruker Daltonik) under mild conditions. Treatment of the Pd^{II} precatalyst with Grignard reagents RMgCl (R = Ph, Bn, Bu) lead to the formation of palladate(II) complexes $[L_nPdR_3]^-$, suggesting a transmetallation reaction. The presence of $[L_nPdR_2–H]^-$ anions implied the operation of C–H activation processes resulting in the loss of RH from $[L_nPdR_3]^-$, which was also observed in gas-phase fragmentation experiments. The main fragmentation pathway of the $[L_nPdR_3]^-$ anions upon CID, however, was the reductive elimination of R_2 yielding the Pd^0 species $[L_nPdR]^-$ (see figure).

These results show that the sequence of transmetallation and reductive elimination is a feasible reduction pathway of the Pd^{II} precatalyst and may play a considerable role in palladium catalyzed cross-coupling reactions.

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Coinage-Metal Ate Complexes – An ESI-MS Study

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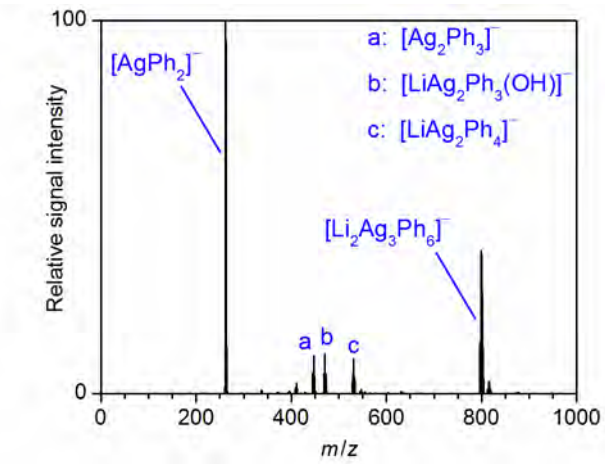

Copper ate complexes are an important class of organometallic compounds thanks to their numerous applications in preparative organic chemistry and, therefore, they have been well studied.[1,2] In contrast, the chemistry of the heavier homologues (silver and gold ate complexes) has not been explored in detail. Electrospray ionization-mass spectrometry (ESI MS) has proven to be a valuable tool for the analysis of charged organo-copper species.[3-5] We applied this method in this work to study organocuprates and their heavier homologues. Solutions of organocuprates, -argentates, or -aurates were prepared by transmetallation of the respective metal cyanide with either RLi or RMgCl in tetrahydrofuran. Standard Schlenk techniques were applied in all cases to exclude traces of moisture. The solutions were diluted and then directly injected into the ESI source of a micrOTOF-Q II mass spectrometer (Bruker Daltonik), which was operated under mild conditions. Negative-ion mode ESI mass spectra of solutions of MCN (M = Cu, Ag, Au) that were treated with organolithium or Grignard reagents showed ate complexes of these three metals with the general sum formula $M_nR_{n+1}^-$ (R = phenyl or methyl). Thus, the three different classes of coinage-metal ate complexes showed far-reaching parallels in their association and aggregation behavior. In addition, heterobimetallic complexes were observed, among which $LiM_2R_4^-$ or $Li_2M_3R_6^-$ were particularly prominent. Upon gas-phase fragmentation, mass selected ions released neutral fragments such as MR, M_4R_4 or $Li_2M_2R_4$.

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ETD experiments on self-assembled asymmetric supramolecular squares

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Introduction:

Mass spectrometry is an essential analytical tool for self-assembled supramolecular aggregates. In addition to the evaluation of stoichiometry, valuable information on relative bond strengths within the weakly-bound aggregate is accessible by fragmentation in the gas phase. We herein present an approach to generate open-shell metallo-supramolecular aggregates by gas-phase one-electron reduction using the electron transfer dissociation (ETD) technique. For this study, we chose four selectively self-assembled asymmetric homo- and heterometallic metallo-supramolecular squares with two different metal corners of the general composition $[\{Pd(\eta^3\text{-2-Me-}C_3H_4)\}_2(L^n{}_2)_4\{M(dppp)\}_2](CF_3SO_3)_6$ [M=Pd, Pt; L_n=4-PPh_2py (L_1); 4-$C_6F_4PPh_2$py (L_2); py= pyridine].[1,2] These intriguing compounds show a variety of potential reduction sites. Their stability as well as the fragmentation behaviour of the mixed-valence reduced product species are addressed.

Experimental

ESI mass spectra were recorded on a LTQ Orbitrap XL™ Hybrid Ion Trap mass spectrometer and an Ion Max source equipped with a Heated Electrospray Ionization (HESI-II) probe. Acetone solutions (100 microM) were transferred into the ion source under soft ionization conditions using the attached syringe pump at flow rates of 5-10 microL/min. A series of multiply charged cations is observed for each species due to abstraction of several anions during the ESI process. For ETD experiments, the ions of interest were mass-selected and treated with fluoranthene in the ion-trap and analyzed in the orbitrap. Fragments of interest were again isolated and fragmented by collision-induced dissociation (CID) to obtain information on stability and fragmentation cascades of the open-shell squares.

Results and discussion

Our previously conducted in depth study on the closed-shell homo- and heterometallic squares with ditopic linkers show that the most important factor determining fragmentation is the type of metal corner and as a second factor the length of the ditopic linker. In CID-experiments, we observe a preference to first cleave the Pd-N bond, followed by the Pd-P-bond and then the Pt-N-bond.

Most closed-shell species in different charge states are easily reduced by electron transfer in the gas phase to yield the intact open-shell species carrying one charge less. The reduced homometallic squares are rather stable and retain the general fragmentation. The heterometallic squares however show a distinct reactivity change upon one-electron reduction. Analysis of the fragmentation cascades indicates the formation of highly reactive Pd(0) via $C_4H_7^{\bullet}$ loss that leads to several C-P bond dissociations either in the dppp-backbone or in the linker. Furthermore proton abstraction from the dppp-backbone by triflate is observed.

ETD-experiments conducted on self assembled asymmetric metallo-supramolecular homo- and heteroleptic squares.

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ETD, metallo-supramolecular-aggregates, one-electron reduction, self-assembly, gas phase reactivity

Formation and structure elucidation of M_2Ag^+ ions with M = [6]helicene, [7]helicene and coronene

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Einleitung

Unsaturated hydrocarbons (e.g. PAHs) are straightforwardly electrospray "ionized" by the attachment of Ag^+ ions. A remarkable feature of the gas-phase interaction of monovalent Ag^+ with molecules (M) is the tendency to react in a bidentate fashion forming M_2Ag^+ ions, commonly be referred to as silver-bound dimers.
This study reports the first time generation of M_2Ag^+ ions with M = [6]helicene and [7]helicene. The [n]helicene is a spiral molecule of "n" condensed benzene moieties. Energy-dependent CID experiments and ion/molecule reactions using the planar coronene as reference, reveal that these M_2Ag^+ ions possess an unusual structure in which one helicene binds one silver in a bidentate way acting as a molecular tweezer, while the second helicene attaches to the first by π-π stacking.

Experimenteller Teil

ESI-MS and -MS/MS (energy-dependent CID) experiments were conducted with a quadrupole time-of-flight instrument (micrOTOF QII, Bruker). For ESI experiments [6]helicene, [7]helicene and coronene were dissolved in dichlormethane/acetonitrile (at typical concentrations of E-05 M) using AgTFA as Ag^+ source.

Ergebnisse und Diskussion

ESI mass spectra of both [6]helicene and [7]helicene show sizeable signals for the "dimeric" M_2Ag^+ ions. This is remarkable, because previous efforts failed to generate such ions [1,2]. The "monomeric" MAg^+ ions are, however, more abundantly observed. The coronene reference molecule produces almost exclusively M_2Ag^+ ions, while MAg^+ ions are hardly observed. This may be taken as a first hint of bidentate helicene binding to Ag^+, which resides between two benzene units of only one helicene molecule acting as a molecular tweezer. This poses the question as to whether or not the "dimeric" $(helicene)_2Ag^+$ ions would still represent the common silver-bound dimers.

The answer is provided by collision-induced ion/molecule reactions. Caused by the tendency to attain two ligands, the mono-ligated Ag^+ ions tend to pick up efficiently residual background H_2O when

subjected to collision processes in quadrupoles or ion traps. This is evident in CID experiments of $(coronene)_2Ag^+$ ions which show for the mono-ligated $(coronene)Ag^+$ fragment ion the efficient H_2O uptake forming $(coronene)Ag^+H_2O$. This reaction is entirely absent when M_2Ag^+ dissociates to MAg^+ with M being a helicene, as the silver resides in the bidentate molecular tweezer.

Energy-dependent CID experiments reveal that loss of one helicene unit from $(helicene)_2Ag^+$ requires tremendously less energy than the loss of one coronene molecule from $(coronene)_2Ag^+$. This indicates that the second helicene ligand in M_2Ag^+ is less strongly connected to Ag^+ than it is the case for coronene. This indicates strongly that the second helicene molecule is connected to the first helicene by π-π stacking (forming Ag^+-helicene-helicene) rather than to a central Ag^+ ion (helicene- Ag^+-helicene is not observed).

These assumptions are confirmed by the observation of a "trimeric" $(coronene)_3Ag^+$ ion, which shows the same energetic ease for the release of one ligand indicating π-π stacking of one coronene to a silver-bound dimer.

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Neue Aspekte: First time observation of M_2Ag^+ ions with M = helicene, possessing Ag^+-helicene-helicene structure.

Stichworte: Ag^+ adducts, helicene, π-π stacking, Energy-dependent CID

Thema: Gasphasenreaktionen & Fragmentierungen

Kategorie: helicene, Ag^+ adducts

Formation and dissociation behavior of multiply charged salt-like cluster ions (sodium formate)

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Einleitung:

Gas-phase cluster are often referred to as the fifth state of matter, possessing properties that lie between the atom and the bulk material, therefore giving further insight into, for instance, the crystallization process. ESI is ideally suited to generate a particular cluster type: the salt-like cluster ion of the form cation(cation/anion-pair)$_n^+$. The formation of these clusters takes place in the ESI source and can be regarded as crystallisation occurring during the evaporation of the solvent. If the cluster increases in size, it becomes possible to accommodate more charges on it, generating multiply charged cluster ions of the form: cation$_m$(cation/anion-pair)$_n^{m+}$. Collision-induced dissociation (CID) performed inside the quadrupole ion trap is a unique way to identify the dissociation pathways of lowest energy requirement.

Experimenteller Teil:

Experiments were performed on an ESI-ion trap (Esquire6000, Bruker Daltonics, Germany) using a direct infusion syringe pump. Solvent mixtures varied, depending on the size and stability of the investigated cluster of interest.

Ergebnisse und Diskussion:

Experiments aimed at the manipulation of the cluster formation process, i.e. influencing the size distribution and the respective intensities of a cluster series of a certain charge state. In particular, the ion source parameters are detailed that lead to efficient formation of cluster ions. Of special interest was it to produce the more labile multiply charged clusters.

In a second set of experiments the decay behavior of the cluster ions was detailed, again the emphasis lay on the di-, tri- and tetracations. The CID behavior of multiply charged sodium formate cluster ions has been investigated before by means of low energy collisions under multiple collision conditions.[2]. However, the unique CID conditions within the quadrupole ion trap as a slow heating resonant excitation device provided much clearer insight into the dissociation processes with only low energy requirement. The multiply charged cluster ions undergo two types of dissociations. These include the loss of a neutral moiety (neutral evaporation) while the cluster ion is retaining its charge and the Coulomb explosion (charge separation), whereby the multiply charged cluster ion dissociates into a pair of fragment ions of a small singly charged fragment ion and the corresponding larger cluster fragment ion with the charge state: m-1. The cluster size variation within different charge states can be characterized by the size-to-charge ratio, r. For the cluster ion: cation$_m$(cation/anion-pair)$_n^{m+}$, the ratio would be: r = n/m. It was found that for intermediate values of the ratio r, both dissociations would occur. However, with increasing r only neutral evaporations would occur beyond a certain limit. Equally, with decreasing r only Coulomb explosion occurs below a certain limit.

Formation and dissociation mechanisms are discussed in light of the magic number behaviour of the cluster ions, identifying ions and/or neutrals that possess geometries of enhanced stability.

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Neue Aspekte:

New insight into fragmentation behavior of multiply charged sodium formate cluster ions by ion trap CID.

Stichworte:

Crystallization, fragmentation behavior, slow heating CID, resonant ion excitation, quadrupole ion trap

Kategorie:

Crystal growth, fragmentation

Wellenlängenabhängige Photofragmentierung von fluoreszierenden Farbstoffen in einem FT-ICR Massenspektrometer

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Bei früheren Untersuchungen wurden Mechanismen der Photodissoziation von fluoreszierenden Farbstoffen analysiert. Dabei entstand die Frage nach der Absorptionsfähigkeit der Farbstoffe bei der verwendeten Wellenlänge in der Gasphase. Es wurde ein durchstimmbarer Farbstofflaser mit einem FT-ICR Massenspektrometer gekoppelt, um die Absorption bei verschiedenen Wellenlängen zu prüfen und in Kombination mit CID mit MS^3-Experimenten weitere Hinweise auf die Mechanismen zu erhalten.

Es wurde ein APEX III FT-ICR Massenspektrometer der Firma *Bruker Daltonik* (Bremen) mit einem 7.05 T Magneten und einer ESI-Quelle verwendet. Die Photodissoziation erfolgte mit durchstimmbaren Farbstofflasern Scanmate von *Lambda Physics* mit 10 Hz im Wellenlängenbereich zwischen 265 nm und 285 nm und LDL von *Laser Analytical* Systems im sichtbaren Bereich. Die Leistung des Farbstofflasers wurde während des Experiments parallel aufgezeichnet. Das Experiment wurde über die Software XMASS *7.0.8* von *Bruker Daltonics* (Billerica) gesteuert. Mit einem neuen Pulsprogramm war ein automatisches Speichern, Durchstimmen der Wellenlänge, sowie das Aussetzen der Lasereinstrahlung nach einer beliebigen Anzahl von Spektren möglich. Außerdem wurde ein Pulsprogramm für MS^3-Experimente geschrieben, bei dem die Vorläuferionen für die Photodissoziation durch Stoßaktivierung (CID) erzeugt wurden.

Es wurden einige Farbstoffe mit Ethyl- und Diethylaminoseitengruppen untersucht. Die Absorption wurde über die Abnahme des Molekülionensignals quantifiziert. Dafür wurden Massenspektren mit und ohne Lasereinstrahlung aber bei gleichem Ablauf des Pulsprogramms miteinander verglichen. Außerdem wurden die Intensitäten der Fragmente miterfasst.
Oxazin 170 ist ein Farbstoff mit zwei Ethylaminoseitengruppen und einer ortho-ständigen Methylgruppe. Im sichtbaren Bereich wurde die Absorption im Bereich von 526 nm bis 576 nm untersucht und nachgewiesen, im UV-Bereich wurde eine Abnahme der Absorption ab 265 nm zu höheren Wellenlängen beobachtet. Die Intensitäten einiger Fragmente variierten mit der Wellenlänge, deshalb wurde das Absorptionsverhalten der intensivsten Fragmente wellenlängenabhängig untersucht. Dafür wurden die Vorläuferionen wellenlängenunabhängig durch CID erzeugt und anschließend durch PD weiter fragmentiert. Dabei wurden weitere Hinweise für die Bildung einer Azarinstruktur nach dem Verlust von C_3H_8 erhalten.
Der Farbstoff Rhodamin 6G zeigte einen Abnahmetrend der Absorption zwischen 268 nm und 282 nm. Im sichtbaren Bereich wurde wie erwartet [1] oberhalb von 520 nm keine Photofragmentierung beobachtet.
Rhodamin B zeigte im längerwelligen sichtbaren Bereich ab 540 nm eine Abnahme der Absorption, bei Wellenlängen oberhalb von 570 nm waren kaum Fragmente sichtbar. Die Abnahme der Absorption in diesem Bereich wurde schon von Jockusch et al. gezeigt [2]. Das intensivste Fragment stammte aus dem Verlust von C_3H_8, der auch an anderen Systemen mit Diethylaminoseitengruppen beobachtet wurde [3].

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Update of an MS/MS Library of NPS for QTRAP® instruments

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Introduction

Since their first occurrence in 2004 Novel Psychoactive Substances (NPS) have swept the European drug market. The EMCDDA has established an early warning system in which over 560 substances, classified into different chemical classes such as phenethylamines, cathinone derivatives, synthetic cannabinoids, piperazines and tryptamines, are currently monitored (1). Due to the fast growing and changing NPS market a spectral library is needed for identification of mass spectrometric data from unknown compounds. The aim of this study was to update the existing MS/MS library developed by Ambach *et. al*, with newly emerged NPS and further to be able to identify substances in seized material (pills, powders, blotters) as well as in blood, using low resolution ESI-MS/MS.

Experimental Methods

Substances were chosen in alignment with the list "Referenzsubstanzen_September_2016" provided by the "Schweizerische Gesellschaft für Rechtsmedizin SGRM"- Fachgruppe Forensische Chemie". Spectra of reference material were recorded following an 8 min chromatographic run on a Synergi Polar-RP column (50 × 2.0 mm, 4 µm) (Phenomenex). MS/MS-spectra were acquired using a QTrap 3200 instrument (Sciex) with positive electrospray ionisation. Enhanced product ion (EPI) spectra were recorded with collision energies 20, 35 and 50 eV and with collision energy spread 35 ± 15 eV. Background subtraction was performed for all spectra before inclusion in the library.

Results and Discussion

The library in its current version contains data for 387 different compounds, including phenethylamines, amphetamines, cathinones, piperazines, synthetic cannabinoids, tryptamines, opioids, designer benzodiazepines, dissociatives, and others including available metabolites. An updated version of the library will come available in April 2017 containing additional 161 substances. Of these 549 substances 280 are scheduled in the Swiss "Betäubungsmittelverzeichnisverordnung, BetmVV-EDI, Anhang e". The MS/MS QTRAP library has an online presence at www.legal-highs.ch. PDF files of spectra for manual comparison and reference will be available online and the database file for the use with the Sciex Analyst software is available for forensic and clinical laboratories from the authors upon request.

This research was sponsored by the Swiss Federal Office of Public Health (BAG project Nr. 15.029013). Substances were generously provided by the "Referenzlabor" at the Forensic Institute Zurich and the Institute of Forensic Medicine Freiburg in the course of the Prevention of and Fight against Crime (ISEC) program of the European Commission (JUST/2013/ISEC/DRUGS/AG/6421).

Neue Aspects

The MS/MS QTRAP library has been updated covering all chemical classes and almost all NPS monitored by the European Monitoring Centre for Drugs and Drug Addiction.

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Keywords:
New psychoactive substances; NPS; library; LC-MS/MS; QTrap;

LC-MS^2 Method Development for Simultaneous Analysis of Antibiotics from Plasma of MDR-TB Patients

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Introduction: Emerging multidrug resistance (MDR) of *Mycobacterium tuberculosis* is a major challenge for the global control of tuberculosis. A long duration of combination antibiotic therapy is necessary to achieve relapse-free cure from MDR-TB. Quantification of antibiotic concentration in plasma plays an important role to offer precisely tailored therapy regimen to patients, referred to as personalized medicine. TDM has the potential to avoid adverse events by enabling the reduction of too high dosages. Low serum drug concentrations have been shown to cause therapy failure and drug resistance where TDM might help to predict treatment outcome and prevent acquired drug resistance. LC-MS/MS is the most suitable method for a multi-analyte assay as is required in the context of TDM.

Experimental: We aim to extract and measure 21 antitubercular drugs in plasma. For application in our clinical setting our panel comprises 17 main second line antitubercular antibiotics: fluoroquinolones (levofloxacin, moxifloxacin), injectables (amikacin, capreomycin, kanamycin), β-lactams (amoxicillin, clavulanic acid, meropenem), and bedaquiline, clofazimine, cycloserine, delamanid, linezolid, PAS, prothionamide, and terizidone. The first line antibiotics rifampicin, isoniazid, pyrazinamide and ethambutol are also included to cover the susceptible TB regimen. Analysis of antibiotics from patients' plasma are performed by using HPLC (Waters Acquity UPLC) interfaced with ESI Triple Quadrupole Mass Spectrometer (Waters Micromass Quattro Premier XE Mass Spectrometer). MS is operated in positive ion mode and the analytes are determined by multiple reaction monitoring (MRM) mode with specific transition parameters optimized for each antibiotic.

Results & Discussion: The main obstacle for establishing a validated LC-MS method with short run time on a single column chemistry, is the structural diversity of the antibiotics. A regular MDR-TB regimen consists of a fluoroquinolone, an injectable and 2-3 further drugs, according to resistance testing. Each of these 5 substances have a different mechanism of action and entirely different chemical properties. Especially diverse hydrophobicity and ionization challenge the development of a single run LC-MS method.

However, the detection of the target compounds by mass spectrometry is successfully established. Masses and mass transition parameters are identified for each of 21 MDR-TB medicines. Every compound had specific and sensitive transition that enables quantitation in MRM mode. The established HPLC-MS method could cover 17 of 21 antibiotics using a HILIC

column. Injectable antibiotics (amikacin, kanamycin, capreomycin) and terizidone requires to be studied further to achieve acceptable chromatographic behavior.

Next steps will be to complete the identification and separation of all antibiotics and to extract the respective antibiotics from patients' plasma. Once operational, the TDM platform will provide possibilities to individualize the dosage of medicines for each patient with MDR-TB in order to optimize treatment outcomes. We have recently started to combine antibiotics levels with lipid metabolite profile in plasma and peripheral mononuclear cells. We found indications that the phospholipids of the inner membrane can help to access the success for pathogen clearance. Targeted quantification of lipids in patient`s blood in correlation to antibiotics level in plasma can help in the evaluation of treatment efficacy.

Novel aspects: LC-MS method for parallel quantitation of anti-TB drugs is established including second line antibiotics.

Keywords: LC-MS, antibiotics, tuberculosis, therapeutic drug monitoring

Modifikation von Papiersubstraten mit hydrophoben Barrieren zur Erhöhung der Empfindlichkeit und Reproduzierbarkeit in der Papierbasierten Massenspektrometrie

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Die papierbasierte Massenspektrometrie (PB MS) hat sich seit seiner Einführung 2010 [1][2] als ein vielversprechendes Ionisationsverfahren bei Atmosphärendruck etabliert und erfährt seitdem reges Forschungsinteresse.
Vorteile der Methode sind der einfache Arbeitsablauf, eine simple technische Umsetzung, sowie die geringen Kosten der verwendeten Papiersubstrate. Zusätzlich bietet die Verwendung von Papiersubstraten den Vorteil eines chromatographischen Effekts, wodurch eine Aufreinigung oder Trennung komplexer Proben ermöglicht wird.
Aufbauend auf den bisherigen Ergebnissen zur Erhöhung der Reproduzierbarkeit der PB MS mittels chemischer Oberflächenmodifikation, erlaubt der neuartige Einsatz hydrophober Barrieren auf den Papiersubstraten, eine Ausbildung stabiler Sprays übe lange Zeiten sowie eine Senkung der Nachweisgrenzen auch unter Verwendung von Wasser als Spray-Solventen. Dies ist eine explizite Voraussetzung für native MS-Untersuchungen und ermöglicht den Einsatz in mikrofluidischen Systemen.
Die hier zusammengetragenen Forschungsergebnisse bilden die Grundlage zur Erhöhung der Empfindlichkeit und Reproduzierbarkeit von PB MS Untersuchungen aus rein wässrigen Lösungen - als Voraussetzung für native MS.
Analog zur Electrospray ionization (ESI) ist bekannt, dass die Ausbildung stabiler Spray-Konen, bei Verwendung von Wasser als Solventen, durch seine charakteristischen Eigenschaften erschwert wird. Dementsprechend verwenden die meisten Arbeiten Solvent-Gemische aus leichtflüchtigen organischen Lösungsmitteln und Wasser. Der hier gewählte Ansatz zur Ausbildung stabiler Sprays sieht die Verwendung hydrophober Barrieren auf den verwendeten Papiersubstraten vor.
Bei der Charakterisierung mittels LIF lassen sich verschiedene Spray-Events beobachten. Es konnte die Ausbildung von Jets, einzelnen Tröpfchen verschiedenen Durchmessers, aber auch von Sprühnebeln beobachtet werden. Die verschiedenen Modi zeigen, dass es sich bei der PB MS um einen erratischen und diskontinuierlichen Prozess handelt. Die Ausbildung der Jets tritt zudem meist an einzelnen Faserenden in der Nähe der Papierspitze auf, wobei unterschiedliche Spitzen zufällige Verteilungen aufweisen und in unterschiedlichen Ausgangspunkten für den Sprayprozess resultieren. Diese Faktoren begründen den Justierungsbedarf jeder neuen Messung und verdeutlichen die mangelnde Reproduzierbarkeit unterschiedlicher Messungen.
Die massenspektrometrischen Ergebnisse zeigten eine deutliche Verbesserung der Spektrenqualität (höhere Analytsignale, bei abnehmenden Hintergrundsignalen), sowie Steigerung der bisher erfassten Sprayzeiten, bei Verringerung der verwendeten Probenvolumina.
Dadurch kann zu Beginn jeder Messung eine „on the fly" Justierung der Papierspitze vorgenommen werden, wodurch die individuelle Verteilung der Faserenden berücksichtigt wird. Weiterhin minimiert die Verwendung hydrophober Barrieren die ungewollte Diffusion des Analyten.
Die in der Literatur dargestellten Auswirkungen solcher Modifikationen auf die Signalintensität sind unterschiedlich.[3][4] Daher wurde der Einfluss verschiedener Größen und Formen der aufgedruckten Wachskanäle untersucht. Sowohl bei gleichen Formen, aber unterschiedlicher Kanalbreiten, also auch bei vergleichbar variierten Kanalformen zeigte sich, dass stärkere Eingrenzungen zu Intensitätsgewinnen führten.
Eine erste Anwendung dieser Kanäle für die Analyse eines Aminosäuregemischs in einer komplexen Matrix konnte die Vorteile wachsbedruckter Papiere bestätigen.

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Characterization of Fast-Pyrolysis Bio-Oil

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Introduction

Crude oil was greatly exploited to meet the increasing demand of modern industry, which creates a harsh pressure on global environment and urgent demand for renewable energy resources. Bio-oils produced from biomass pyrolysis show great potential to be used as an attractive substitute. Detailed understanding of its composition allows researchers to optimize pyrolysis conditions and improve upgrading techniques, and thus make bio-oil production more cost-effective. Currently, negative ESI ion mode is widely applied for bio-oil characterization in mass spectrometry, however, other ionization methods are less commonly used. Also single ionization technique cannot achieve complete picture of complex bio-oil composition due to limited ionization efficiency. Therefore, multiple ionization techniques will be considered to get a better understanding of bio-oil composition.

Experimental

A liquid bio-oil was prepared by fast pyrolysis at temperature of 500 ^{o}C using a short residence time < 2s and then condensed by ice bath. For analysis, bio-oil was diluted to a final concentration 250 ppm with MeOH:Tol (1:1 v/v) for ESI(+), APPI and APCI and ACN for ESI(-). MS measurements were performed on an research-type Orbitrap Elite at a resolving power of 480,000 (FWHM at 400 Da) using the spectral stitching method (windows of 30 Da with 5 Da overlap). Ionizing was performed using ESI (in positive and negative mode), APCI and APPI(10.0/10.6 eV). Data analysis was processed using Composer v1.50 (Sierra Analytics, Modesto, CA, U.S.A.).

Results

Bio-oil is a complex mixture containing thousands of organic, mostly oxygen–rich compounds (carboxylic acids, phenols, alcohols, aldehydes, ketones, ethers, esters, furans, sugars, and water) derived from cellulose, hemicellulose and lignin (the most abundant species) in biomass. In the negative ESI mode, a wide range of O_x species was discovered containing up to 20 oxygen atom. Additionally a broad range of NO_x and SO_x species was also identified. The compounds DBE (Double Bond Equivalent) distribution analysis somehow indicates the origin information of pyrolysis products. Chemically, lignin are cross-linked phenolic polymers, however, cellulose, hemicellulose are more likely to be saturate compounds. Therefore, pyrolysis products from lignin (phenolic compounds) show high aromaticity, which contain a wide range DBE distribution starting with DBE 4 in comparison with compounds from cellulose and hemicellulose. According to ion abundance of $O_{2\text{-}10}$ classes, DBE decreases from 2 to mostly 3~4, and then increases to reach the top again at around 5~6, which implicates a clear distinction between sugaric and phenolic compounds. For the positive ESI mode, NO_x, SO_x species are the most abundant species, which are more basic than those identified in ESI negative mode, ensuring them to receive a proton in protic solvent. Here,O-species with up to 7 oxygens are observed. In APPI&APCI, both radical and protonated cations can be observed with 3309 compounds in total being identified as radical cation and 9716 as protonated cation, separately. Most of the elemental compositions (3114, above 94%) found as radical cations were also discovered as protonated cations. O_x-species are the highest abundant species in the bio-oil.

New aspects

Through complementary analysis using multiple ionization techniques, a better understanding of bio-oils can be achieved and exploited for future studies.

Characterization of a New Extractive Electrospray Ionization (EESI) Source for Online Particle Analysis and its Application to Atmospheric Aerosol

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Introduction (max 120)

To assess particle composition, current particle measurement techniques struggle to efficiently shift analytes from the condensed phase to the gas phase for mass spectrometric analysis at a molecular level. Thermal desorption of aerosol components for gas phase analysis is typical in most online aerosol sampling instruments, but thermal decomposition during desorption even at low temperatures (<100 C) can significantly alter the measured composition. Even instruments that utilize soft ionization techniques still rely on some type of thermal desorption to evaporate material into the gas phase for analysis; and therefore suffer from changes in particle composition in unpredictable ways due to decomposition. Therefore there remains a fundamental need for online, rapid-response chemical characterization of particles without artifacts from thermal decomposition.

Experimental Section (max 120)

The design and the characterization of the online extractive electrospray ionization (EESI) source, recently developed at TOFWERK in collaboration with the Paul Scherrer Institute (PSI) will be presented. All measurements were carried out on a chemical ionization atmospheric pressure interface time-of-flight mass spectrometer (CI-API-TOF, *TOFWERK*), an efficient, compact, and field deployable high-resolution time of flight mass spectrometer. It will be shown that using this ionization source yields a fast molecular analysis of aerosol organics without heating induced fragmentation. The instrument is also capable of nano-particle analysis (particle diameter < 50nm). We describe the ionization source, its characterization, and application to atmospheric aerosol composition as proof of concept measurements both in atmospheric simulation chambers and ambient field measurements.

Results and Discussion (max 300)

We use results from the reaction of α-pinene and ozone as a diagnostic reaction system to assess the performance of the EESI-TOF. This system provides a challenging test case as the reaction leads to the prompt formation of a suite of molecular dimers in the gas phase, which have traditionally been impossible to measure in real time in the condensed phase, due to their extremely low volatility and propensity to undergo thermal decomposition. Using an atmospheric simulation chamber at PSI we demonstrate that the EESI provides rapid response (1 Hz) measurements of highly oxidized organic species and oligomers with individual compound detection limits as low as 1 ng m^{-3} in 5 seconds, allowing for the simultaneous retrieval of molecular composition for hundreds of compounds that comprise the organic aerosol at high time resolution.

We present a detailed instrument characterization demonstrating linearity, a lack of matrix effects or water vapor dependence, the ability to measure particles as small as 20 nm, and present progress towards parameterized sensitivity for unknown compounds observed in the mass spectrum for which standards do not exist. We discuss the complete instrument setup in the context of current aerosol

measurement shortfalls, and potential applications of the source to the chemical speciation of organic and inorganic aerosol at atmospherically relevant conditions.

Novel aspect (max 20)

We present the first online ionization of ambient nano-particles at ~ng m^{-3} concentrations by extractive electrospray ionization mass spectrometry.

References (max 5)

Keywords (max 5)

Nano Particle Analysis, Extractive Electrospray Ionization, Online Analysis

Characterizing the LILBID ionization method: energy transfer and dissociation

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Laser-induced liquid bead ion desorption (LILBID) is a native mass spectrometry ionization method particularly valuable in elucidating the stoichiometry of noncovalent biomolecular complexes. In this method, 30 µm or 50 µm droplets of aqueous sample are irradiated with infrared light, causing the droplet to explode and release ions. In establishing this new method, we pose two related questions: how much energy do ions receive during desorption and how much dissociation is caused by the ionization process? Knowing that softer or harsher laser settings result in intact or dissociated complexes, we also seek to understand the correlation between laser settings and dissociation. The softest laser settings may contribute negligible energy, resulting in spectra which reflect the solution state.

Experimenteller Teil

To address the first question, the pulsed acceleration voltages were set to select ions moving at certain velocities post-explosion. By varying the velocity ranges selected and integrating the resulting signal intensities, approximate velocities of ions post-explosion were determined. To determine how much dissociation occurs during ionization, double-stranded DNA was run at different temperatures and the percent of duplex calculated from each spectrum, yielding a LILBID-based melting curve for comparison with a UV-vis melting curve. The RNAse A/5'-CTP complex was run on LILBID, and the dissociation constant obtained from the spectra was compared to literature values. Finally, a workflow was established to investigate the interplay between droplet position relative to the laser beam, laser energy absorbed, and dissociation seen in spectra.

Ergebnisse und Diskussion

Following desorption, Cs+ ions had a velocity range of approximately 4-48 km/s. However, since this initial experiment was conducted using the Cs+ peak from CsI spectra, the dissociation of CsI clusters is a serious confounding factor in being able to calculate a relevant energy distribution from these data. Further studies with non-aggregating and non-fragmenting small molecular or atomic ions will use the same setup to evaluate total energy after laser desorption as a function of laser settings. Melting curve studies with double-stranded DNA yielded a melting point of 40.5C at maximal laser power compared to the 52.3C obtained from UV-vis spectroscopy. This decrease in the apparent melting point can be explained by the introduction of laser energy to the system. This shift could be decreased by altering laser settings. Ultimately, the goal is not only to quantify this shift so that unknown binding affinities can be calculated from LILBID spectra but also to characterize its dependence on laser settings and to find laser settings to minimize the shift. Thus the solution state could, in effect, be observed directly with LILBID. In initial studies with the RNase A/5'-CTP complex, movement of the droplet relative to the laser beam was a source of error and of lack of reproducibility. Nevertheless, LILBID spectra yielded dissociation constants between 0.01 and 8.5 µM, in a reasonable range compared to nESI, circular dichroism, and calorimetry-based literature values between 0.5 µM and 2 µM. Future experiments with both small ions and biomolecular complexes will incorporate the new workflow that takes into account droplet position relative to the laser beam. This should simultaneously address the

problem of reproducibility encountered in the RNase A studies and yield information on how droplet position affects the amount of energy received by ions during desorption.

Neue Aspekte

Understanding energy transfer in the LILBID process; relating dissociation in LILBID spectra to dissociation in the solution state.

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Analysis of Liquid Crystal Display Sealants using Spatially Resolved Mass Spectrometric Methods

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Introduction (max. 120)

Liquid crystal displays (LCDs) are the most established flat-panel displays for TV screens, laptop computers and mobile phones.[1] The operation mode of these displays is based on the alignment of a liquid crystal (LC) mixture when applying an electrical field. Organic and inorganic contaminations in the LC layer can cause display defects.[2] A possible source for those contaminations is the display sealant, which adheres to the two glass substrates containing the LC layer. The sealant is a mixture of two polymerizable components, which are cured with UV light and heat.[3] The designated aim of this project was the spatially resolved detection of LCD sealants on display samples and the differentiation from the LC to detect possible sealant contaminations.

Method (max. 120)

For the molecular investigation of the sealants, the combination of laser ablation with atmospheric pressure chemical ionization mass spectrometry (LA-APCI-MS) was used. The hyphenation of LA-APCI-MS was first established by HERDERING *et al.* in 2013 and offers the possibility to analyze the distribution of various molecules in solid samples without time-consuming sample preparation.[4] To further improve the identification of possible sealant contaminations in the LC layer, a principle component analysis (PCA) was performed for five different LCD sealant samples, two LC mixtures and three display samples. For a multimodal spatially resolved approach, the sealants were also analyzed by means of laser ablation-inductively coupled plasma-mass spectrometry (LA-ICP-MS) to identify characteristic elements in the sealant.

Results and discussion (max. 300)

For LCD sealants, aromatic acrylates are often used as UV-curable compound and epoxy resins like Bisphenol A diglycidyl ether are used for heat curing. By means of LA-APCI-MS, characteristic sealant fragments were identified and characterized. A spatial

resolution down to 100 µm was achieved for the ablation of single lines of various display samples and the sealant edge could be clearly distinguished from the LC layer for all investigated samples. Moreover, it was possible to identify some sealant ions as Bisphenol A diglycidyl ether fragments by comparison with a standard material. With the help of the principle component analysis, sealants and LC mixtures as well as display samples could be classified correctly. Moreover, it was possible to differentiate between the two different LC mixtures.

By means of LA-ICP-MS, nickel, zinc and gold were detected and further investigated. Especially the occurrence of gold is noteworthy, because it is rare in the manufacturing process of LCDs and can easily be assigned to sealant contaminations in the LC layer. The origin of gold in different sealant samples could not be clarified by now. In contrast to gold, nickel and zinc are more frequently used in the manufacturing process. Thus, nickel and zinc signals in the LC layer cannot be definitely assigned to sealant impurities. Despite this, the identification of the sealant edge on display samples could be verified with the additional LA-ICP-MS approach.

New aspects (max. 20)

For the first time, LA with molecular and elemental mass spectrometry was applied for the spatially resolved analysis of LCDs.

Keywords (max. 5)

liquid crystal display, sealant, laser ablation, APCI-MS, ICP-MS

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Determination of multi-element composition and mass of single nanoparticles in liquids and air

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The list of analytical techniques which can be applied for nanoparticle detection in complex media and at low environmentally relevant concentrations (ppt-ppb) is very short and for most of the studies complementary approaches are considered. Single particle (sp)-ICP-MS provides an easy and routinely applied way to quantitatively determine size and number concentration of metal-containing nanoparticles. Moreover, element-specific detection makes sp-ICP-MS more tolerant to high levels of natural background.

Along with size and concentration, multi-element composition of single nanoparticles is extremely valuable to study chemical transformations of particles once they have entered the environment. Besides, composition of single particles can be used as a specific merit for the identification of synthetic nanoparticles in the presence of naturally occurring particulate background and for particle source tracing.

Experimenteller Teil

All ICP-MS measurements were carried out on a TOFWERK *icp*TOF in combination with either the standard liquid introduction system or a gas exchange device (GED) and the the metal standard gas generator (MSGG) for atmospheric aerosols. Nanosteel particles were supplied by NanoDefine project and measured in liquid dispersion. Standard reference material urban particulate matter NIST 1648 suspended in a gas sampling bag with nitrogen was used for the validation of single particle ICP-MS method in the gas phase. Car exhaust was sampled outdoor into the gas sampling bag and measured 10 minutes after sampling.

Ergebnisse und Diskussion

In this study we compare different methods for quantification of elemental composition and mass of single particles in both aqueous media and in air using the icpTOF. The TOFWERK icpTOF mass spectrometer allows for detection and quantification of all isotopes in single particles. Different calibration approaches were validated using synthetic nanosteel particles in water and urban particulate matter from NIST suspended in air. Multi-element sp-icpTOF-MS enabled accurate assessment of multi-element composition of nanosteel. Two aerosol calibration methods for atmospheric aerosols gave very similar results for the NIST standard with recoveries in the range of 67-140%. Ir and Pt particles detected from the car exhaust were in the nano-size range with the ratio of Pt/Ir varying from 0-10 and are most likely the emission from catalytic converter.

Neue Aspekte

New methods for multi-element analysis of single particles from complex samples are presented and validated in this work.

Molecular laser ablation-mass spectrometry for rapid identification of synthetic cannabinoids

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Einleitung

Synthetic cannabinoids as replacements for Δ9-tetrahydrocannabinol pose an increasingly problematic issue for both legal classification and forensic analysis. These compounds bind to the cannabinoid receptor in the human body, leading to a similar intoxication as conventional Δ9-tetrahydrocannabinol.[1] Once a synthetic cannabinoid has been classified as illegal by incorporating it into federal law, its prohibition can be circumvented by small changes to the molecular structure. This leads to a large variety of different synthetic cannabinoids on the market, the toxicological effects of which are often unknown. Furthermore, it is not possible to detect new substances via conventional drug testing techniques such as immunoassays.[2] Chromatography-based methods (LC-MS, GC-MS) are state of the art but time consuming and require a complex method development.

Experimenteller Teil

Laser ablation (LA) -atmospheric pressure chemical ionization (APCI) coupled to high resolution mass spectrometry (HR-MS) provides a fast method to identify different types of synthetic cannabinoids on herbals, often used as carrier material, within a single measurement. For this purpose, the samples are placed contiguous to each other in the ablation chamber of a laser ablation system without any further sample preparation. Small amounts of sample material are ablated consecutively from each of the samples by a Nd:YAG laser (213 nm wavelength), employing a single line scan across all of the samples.

Ergebnisse und Diskussion

A representative mass spectrum for each sample is obtained, thus enabling the identification of the analyte through accurate mass and the substance-specific fragmentation pattern. Moreover, HR-MS is a versatile tool to identify unknown synthetic cannabinoids that enter the market in future.
Using this technique, three different analytes were successfully identified within a total measurement time of only 1.6 minutes. LA-APCI-MS therefore provides a fast identification method for drug analysis without sample preparation and significantly shorter measurement times than commonly used techniques such as LC-MS or GC-MS.

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Neue Aspekte (max. 20 Wörter)

A rapid identification method for synthetic cannabinoids was established, providing short measuring times without sample preparation.

Albumin adducts as biomarkers of an exposure with organophosphorus pesticides

Jens von der Wellen, Horst Thiermann, Harald John

Introduction:

Causing approximately 300.000 human poisonings per year, pesticides account for a third of all suicides worldwide. The majority is attributed to organophosphorus pesticides.[1,2] They inhibit the pivotal enzyme acetylcholinesterase via covalent binding, resulting in an accumulation of the neurotransmitter acetylcholine at nicotinic and muscarinic synapses. This may lead to severe neuronal symptoms and, if untreated, to death by respiratory arrest.[3]

A systematic analytical verification method to prove organophosphorus pesticide poisoning was developed focusing on albumin adducts. An essential advantage of this method is that albumin adducts in comparison to other biomarkers like adducted butyrylcholinesterase have a longer half-life of approximately three weeks which enables detection over a longer period.[4]

Experimentals:

Human serum albumin (HSA) and serum were incubated with the pesticides paraoxon-ethyl and parathion-ethyl *in vitro*. After separation of proteins via precipitation with acetonitrile or ultrafiltration the albumin-fraction was treated with the proteases pronase, pepsin or trypsin separately. Resulting peptides or amino acids containing the phosphorylated tyrosine residues 411 and 138 were analyzed via microbore liquid chromatography-electrospray ionization high-resolution tandem-mass spectrometry (µLC-ESI MS/HR MS). Method optimization included e.g. elaboration of MS/MS-parameters, concentration of pepsin and trypsin and time of proteolysis. The limit of detection was determined and applied to *in vitro* samples of other pesticides and real samples of a patient.

Results and Discussion:

Treatment with pronase lead to a single phosphorylated tyrosine residue. Cleavage by pepsin resulted in the albumin-derived peptides LVRY^{411}TKKVPQVSTPTL and VRY^{411}TKKVPQVSTPT. Proteolysis with trypsin yielded the peptides Y^{411}TK and Y^{138}LYEIAR.

Optimum incubation time for maximum yield of the phosphorylated products was 2 h (pronase and pepsin) and 5 h (trypsin). Best suited pepsin:protein ratio was 1:128 and the optimum trypsin:protein ratio was 1:50. For each peptide MS/MS-parameters like ionization spray voltage floating, collision energy and declustering potential were optimized. Furthermore, stability of the phosphorylated cleavage products was shown over 24 h while storage in the autosampler at 15 °C. Phosphorylated albumin itself proved to be stable at 37 °C (body temperature) and at -30 °C (storage temperature) over a period of 27 days.

The limit of detection varied between an incubation concentration of 0.25 µM paraoxon-ethyl (phosphorylated tyrosine) and 64.0 µM (peptide Y^{138}LYEIAR). Interspecies comparison showed differences in the yield of the phosphorylated products between individuals of one species, but also between different species. This was presumably due to differing concentrations of paraoxonase 1 (PON1), which is known to hydrolyze paraoxon. Differences were also found after incubation of serum and HSA with different pesticides indicating different reactivities with the tyrosine residues 411 and 138. Plasma samples of a patient who was poisoned with pirimiphos-methyl showed a half-life of 37 h of the HSA-adduct with pirmiphos-methyl. The fast degradation was presumably due to oxime therapy.

New aspects:

A systematic method for the detection of albumin adducts with organophosphorus pesticides was developed, optimized and applied to real samples.

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Keywords:

pesticides, organophosphates, mass spectrometry, biomarkers, albumin adducts

Identification of oxidative biomarkers in synovial fluid of patients suffering from rheumatoid arthritis

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Introduction

Reactive oxygen species (ROS) can damage biomolecules in organisms either by direct oxidation or indirectly reactive molecules formed by oxidation, such as dicarbonyls. These non-enzymatic posttranslational modifications (PTMs) have been correlated to several diseases, such as chronic inflammation, heart failure, and cancer. These PTMs are very diverse and usually present in very low concentrations, but they are assumed to alter the structures of proteins and thus their functions.

Rheumatoid arthritis (RA), which mainly affects joints, is an inflammatory, systemic autoimmune disease. The underlying disease mechanisms have been only partially revealed. RA development is characterized by chronic inflammation and associated with increased ROS production. Thus, protein oxidation can serve as a valuable biomarker for monitoring disease development and progression.

Experimental section

Synovial fluid samples collected from RA patients and a control group were digested with trypsin. Samples were purified by solid phase extraction (SPE), separated by nanoRP-HPLC and analyzed on a nanoESI-Orbitrap-LTQ-MS. Modified peptides typically present at low quantities were identified by a combination of consecutive data-dependent acquisition (DDA) methods based on exclusion (all unmodified peptides) and inclusion lists (peptides with significant differences between RA and control sample groups).

Results and discussion

The classical DDA workflow identified more than 1400 unmodified peptides representing 226 synovial fluid proteins with high confidence scores using Sequest search engine. Due to the DDA bias towards highly abundant unmodified peptides and lowly abundant modified peptides in biological samples, less than 600 oxidized peptides were identified. Thus, unique *m/z*-values and retention times of unmodified peptides were used in an exclusion list to overcome these limitations. This allowed to identify 1300 peptides containing sixteen different modifications, such as oxidized arginine, threonine, proline, and lysine, eight different lipid peroxidation products (LPPs), and four modifications related to glycation. Signal intensities of the modified peptides varying between RA and control samples were used to define a set of 41 peptides that could discriminate between disease and control samples. For instance, hydroxy-hexenal-derived modifications on cartilage oligomeric matrix protein (COMP) and proteoglycan 4 were specific for RA samples and representative cartilage proteins. The set of modified peptides from cartilage proteins might be useful to identify reliable RA-specific biomarkers using larger collections of patient and control samples.

Novel aspects

Identification of PTMs in synovial fluid of RA patients provides more detail about the disease.

Keywords

Rheumatoid arthritis, mass spectrometry, oxidative stress, post translational modification

Mass spectrometric investigation of N-acetylcysteine as a potential scavenger against sulfur mustard

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Introduction

The vesicant sulfur mustard (SM) is a banned chemical warfare agent for which no causal therapy exists.[1] Therefore, research for antidotes and scavengers against SM is of high interest. The toxicity of SM is assumed to be due to the alkylation of proteins and DNA.[2] Consequently, substances with a scavenging effect should inhibit such alkylation processes. One potential scavenger is N-acetylcysteine (NAC). NAC is already administered to mitigate symptoms of SM intoxication due to its anti-inflammatory effects.[3] However, it is still unclear, whether beneficial effects are only due to physiological processes or also due to chemical scavenging.[4] Therefore, aim of this study was to investigate the influence of chemical scavenging of NAC towards SM under physiological conditions.

Experimental

Human serum was mixed simultaneously with NAC in different concentrations together with a fixed concentration of SM to characterize the potential of NAC preventing protein alkylation. After addition of acetonitrile the precipitated protein fraction was separated from small molecules in the liquid phase. Proteins were proteolyzed using proteinase K (ProtK). Resulting peptides and small molecules of the liquid phase were analyzed using microbore liquid chromatography-electrospray ionization high-resolution tandem-mass spectrometry (µLC-ESI MS/HR MS). Furthermore, degradation kinetics of SM in phosphate buffered saline (PBS) were examined in presence and absence of NAC. At defined time points aliquots of the respective SM solutions were added to human serum albumin (HSA). Following proteolysis, samples were analyzed via µLC-ESI MS/HR MS to monitor HSA-SM adducts.

Results and discussion

HSA is a well-known biomarker for SM exposure. Its Cys^{34} residue containing a free thiol-group forms stable adducts with SM and NAC. Recently, we have introduced novel analytical methods to detect HSA-SM adducts.[5] After proteolytic cleavage of the HSA adduct with ProtK the SM-alkylated tripeptide hydroxyehtylthioethyl-CysProPhe (HETE-CPF) or the disulfide-bridged NAC-CysProPhe (NAC-CPF) products were obtained. Although, a portion of NAC was alkylated by SM under physiological conditions, NAC did not reduce the amount of HSA-SM adducts independent of its concentration. Two major reaction products of NAC and SM were identified and characterized by µLC-ESI MS/HR MS using collision-induced dissociation (CID). Moreover, kinetic measurements clearly demonstrated that NAC did not increase the degradation velocity of SM when compared to simple aqueous hydrolysis in PBS. Therefore, we conclude that NAC does not diminish SM concentration by chemical scavenging. Accordingly, beneficial therapeutic effects observed under NAC therapy might be due to physiological effects like scavenging of radical oxygen species, stimulation of glutathione production or anti-inflammatory effects. Nevertheless, to the best of our knowledge we herein present disulfide-bridged NAC-CPF adducts for the first-time. Furthermore, this analytical procedure can easily be transferred to test other therapeutics for their scavenging potential against SM *in vitro*.

New aspects

Even though reaction products of NAC and SM were detected and characterized, chemical scavenging did not reduce albumin alkylation.

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Keywords

Sulfur mustard, N-acetylcysteine, high-resolution mass spectrometry, scavenger, albumin adducts

The role of mass spectrometry in the identification of autoantigens as targets in neurological autoimmune diseases

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Introduction: In neurological autoimmune diseases, the nervous system is attacked by immunoreactions. For the diagnosis, anti-neuronal autoantibodies are analyzed. The test systems contain the corresponding target antigens, which first have to be identified. Here we present an indirect immunofluorescence assay (IFA)-based antigen identification strategy consisting of different immunoprecipitation (IP) protocols, mass spectrometry (MS) and IFA with recombinant cells.

Methods: Sera and CSF of patients suspected of suffering from an autoimmune neurological syndrome were comprehensively investigated for the presence of anti-neuronal IgG autoantibodies by IFA using brain tissue cryosections and established recombinant neuronal antigen substrates. Samples showing an autoantibody reaction with brain (rat and monkey cerebellum or hippocampus) but reacting negative in established monospecific assays were subjected to an IFA-based immunocomplex solubility assay to determine the most suitable method: either using cryosections (histo-immunoprecipitation, HIP) or whole tissue lysates (tissue-immunoprecipitation, TIP). HIP or TIP eluates were subsequently analyzed by SDS-PAGE and MALDI-TOF/TOF MS after in-gel tryptic digestion. Identifications were confirmed by recombinant expression of the respective antigen in HEK293 cells, which were used as substrates for IFA and antibody neutralization assays.

Results and Discussion: So far, more than 20 different autoantigens, most of them unknown, could be revealed out of 245 patient samples. Among the novel autoantigens, Inositol 1,4,5-triphosphate receptor type 1 (ITPR1) [1], Neurochondrin (NCDN) [2], and Sodium/potassium-transporting ATPase subunit alpha-3 (ATP1A3) [3] were identified. All new antigen candidates could be verified as target antigens. The recombinant cell-based IFA substrates produced for verification could be readily used in serology such that the clinical value of the autoantibodies was rapidly evaluated in cohort studies. The presented antigen identification approach offers a hypothesis-driven instrument for identifying unknown autoantigens and contributes to a better diagnosis of autoimmune diseases.

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Proteomic investigation of skin cell layers by tissue ablation using picosecond infrared laser (PIRL)

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Skin anatomy, protein structures and their functions are established and explored in great part. Nonetheless, the protein composition in each type of cell layers of skin – particularly in the five different cell layer types in epidermis - are not accurately defined. Therefore, we have undertaken a proteomic approach by using an innovative, in "one-step" extraction and homogenization method, called DIVE (desorption by impulsive excitation) of intramolecular vibrational modes of water molecules in the cell by absorption of laser irradiation in the wavelength at 3 µm. The pico-second infrared laser (PIRL) radiation leads to blast biomolecules out of tissues on pico-second timescale in the gas phase. Furthermore, we tried to find out if PIRL can replace the conventional homogenization methods[1,2].

Experimenteller Teil

Mechanically separateddermis and epidermis of skin biopsies were ablated using PIRL radiation as well as homogenized with conventional tissue disruption methods. For lysis procedure two different buffer system were verified, 8 M urea buffer, and 1% w/v SDC (sodium deoxycholate) buffer containing 0.1 M TEAB (triethylammonium bicarbonate). The collected proteins were reduced with dithiothreitol and the cysteines were alkylated with iodoacetamide. Finally, Trypsin were added and the digestion was performed overnight. Tryptic digested peptides were subjected to a nano-UPLC-ESI-MS/MS using a hybrid quadrupole orbitrap system (Q Exactive, Thermo Fisher scientific) and a Tribrid mass spectrometer (Orbitrap-Fusion, Thermo Fisher scientific). Data analysis was performed with Proteome Discoverer 2.0 (Thermo Fisher scientific) against the UniProt human database.

Ergebnisse und Diskussion

Due to the wavelike structure and different thickness of epidermis within a small area, the proteome analysis of skin suffers. The aim of this study was to establish a method for protein identification and characterization of different cell layer types of skin tissues and finding typical protein markers for those defined layers. The first step to reach this issue is: creation of a skin proteomes library based on an experimentally performance as well as available data bases. A combination of conventional methods and PIRL homogenization method allow to catch a large number of proteomes and proteome isoforms. We could identify more than 2500 proteins identified with unique peptides ≥2 in epidermis an 1200 proteins in dermis. The Less identified protein IDs in dermis were probably caused by the complex meshwork of highly cross-linked protein fibers in dermis which occasion the strength, extensibility and elasticity of dermis and the extracellular matrix which needs an additional enrichment step.

Using two different types of lysis buffer for data base creation benefits to heighten the range of proteins by their different physicochemical properties. The results shown 65 % of proteins

are found in both buffer system whereas 35 % of proteins were found distributively in SDC or urea buffer.

The identified proteins by mass spectrometric analysis were compared to the literature and a protein catalogue were generated for each layer - epidermis and dermis - by validation with "The Human Protein Atlas"[3], which was used for finding epidermal and dermal markers by studying of immunohistologies of skin tissues.

The investigation of skin proteomics layer by layer is complicated not only by unevenness of skin structure but also by age and type of skin biopsies. Therefore, this approach requires more detailed optimization of the level of tissue type and age.

Neue Aspekte

3D ablation with visualization using optical coherence tomography (OCT)

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*** Titel des Beitrags**

N-Acetyltaurine as a novel urinary ethanol marker in a drinking study

*** Einleitung (120)**

To prove alcohol abstinence, various direct alcohol markers are currently analyzed in different matrices such as hair, urine and blood. The most prominent markers are ethyl glucuronide (EtG), ethyl sulfate (EtS) and phosphatidylethanol, representing the non-oxidative pathway of ethanol metabolism. N-Acetyltaurin (NAcT) was found to be an alcohol related, direct marker which is part of the oxidative pathway of ethanol metabolism during a study with mice[1]. NAcT is formed when the oxidative metabolites of ethanol oxidation, acetate or acetyl-CoA, react with the non-proteinogenic amino acid taurine. We investigated the increase in NAcT in human subjects during a drinking study with eight subjects and compared the urinary increase with the well-established marker EtG, EtS and the increase in blood alcohol concentration.

*** Experimenteller Teil (120)**

A ZIC-Hilic based LC-MS/MS method was developed and validated to simultaneously measure creatinine and NAcT in human urine samples obtained during a drinking study. The urine's dilution was corrected by normalization to a creatinine concentration of 1 mg/mL. During the drinking study, blood and urine were taken every 1.5-2 h from eight subjects who ingested 0.66 to 0.84 g/kg alcohol to reach a target blood alcohol concentration of 0.8 g/kg. The results for NAcT could be directly compared to EtG and EtS in urine, measured with a reversed phase LC-MS/MS method, and the blood alcohol concentration, measured with GC-FID.

*** Ergebnisse und Diskussion (300)**

NAcT was found to be an endogenous substance which was present at a range of 1.0 to 2.3 µg/mL in the urine of alcohol-abstinent subjects. Following alcohol ingestion, NAcT concentrations increased in all subjects within 3 to 6 hours to reach a mean peak NAcT concentration of 14±2.6 µg/mL (range 9-17.5 µg/mL). Within 24 hours, NAcT concentrations reached endogenous levels again. Compared to the blood alcohol concentration, NAcT concentrations were found to be slightly shifted. When BAC was not detectable anymore, NAcT levels were still elevated. In contrast to NAcT, the two established markers EtG and EtS have the advantage of being undetectable when no alcohol was consumed, which simplifies the interpretation of the result. So far, the analysis of NAcT concentrations shows no advantage when compared to EtG or EtS analysis. However, it can serve as a further indication for alcohol consumption.

*** Neue Aspekte (20 Wörter)**

First drinking study to investigate the potential of the novel urinary ethanol marker NAcT in human subjects.

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Differentiation and Identification of Explosives Formulations by Means of HPLC-MS

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Einleitung

Forensic scientists constantly develop improved methods for the detection and identification of hazardous materials employed by criminals and terrorists. In this field, explosive compounds are of particular interest, due to their destructive potential. The identification of confiscated explosives that do not appear to be homemade is of importance to uncover and reveal distribution pathways of these materials. Commercial explosives formulations pose highly complex matrices, which do not allow for a straight forward sample preparation and analysis. Earlier approaches therefore mainly focused on a few selected compounds, in order to identify these complex mixtures.[1] More recently powerful statistical methods have enabled scientists to identify pronounced differences between a great amount of samples, while taking into account more data.[2]

Experimenteller Teil

Reversed phase high performance liquid chromatography (RP-HPLC) in combination with high resolution mass spectrometry (HR-MS) was employed to analyze and differentiate commercially available, PETN based explosives. Dispersive extraction of analytes from several different explosives formulations allowed for a reduction of sample complexity.

Ergebnisse und Diskussion

Several commercial explosives were analyzed in regard to their composition with focus on byproducts and additives. Molecular formulae for various additives and byproducts could be derived from exact masses, taken from HR-MS spectra. Although the predominant species were derivatives of PETN, including products of hydrolysis and dimerization, the presence of additives, which are not related to PETN, could be shown as well. Since pronounced differences in the amount and character of byproducts, as well as additives, between the samples could be shown, a differentiation of the samples was possible.

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Neue Aspekte

A new method for the identification of explosives was developed, which relies on a widely implemented and widespread instrumentation.

Stichworte

Explosives, HPLC, HR-MS

Separation of isomeric cannabinoids by high-resolution ion mobility-MS for the differentiation of legal and illegal marijuana

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Introduction: Δ^9-Tetrahydrocannabinol (THC) and cannabidiol (CBD) are two isomeric cannabinoids present in marijuana. CBD lacks the psychoactive effects of THC, but possesses pharmacological activity which is explored for therapeutic applications. In Switzerland, only plant material with a THC content of 1% or higher is controlled by the narcotics legislation. High-CBD/low-THC marijuana products can be legally sold. However, legal CBD- and illegal THC-marijuana cannot be reliably distinguished by appearance or smell, but only by forensic chemical analysis of organic extracts thereof. This is usually achieved by GC- or LC-based techniques. We investigated the suitability of ion mobility-MS as an alternative method for the analysis of THC and CBD as well as their biogenetic carboxylic acid precursors ("-acid-A").

Experimental: Dried plant material (500 mg) was grounded and extracted with 10 mL methanol:*n*-hexane (9:1, *v*/*v*) by ultrasonication. Extracts were diluted 1:100 with methanol and analyzed on a TOFWERK IMS-TOF comprising an ESI source, a 10 cm desolvation tube, a 20 cm drift tube (both made from resistive glass) and a HTOF-MS. Desolvation and drift tube were thermostated to 60°C with nitrogen as the buffer gas. Ion mobility separation was carried out at reduced field strengths of ca. 2 Td. Drift-tube pressure was set to 1000 mbar (nitrogen). Measurements were carried out in both positive and negative ion mode (applied potential approx. 2 kV). Raw IMS-TOF data was analyzed using the Tofware post-processing software.

Results and discussion: The isomeric cannabinoids CBD and THC as well as their precursors CBD-acid A and THC-acid A can be directly ionized from organic solution by ESI. We could achieve baseline separation of CBD/THC (in positive mode) and CBD-acid A/THC-acid-A (in negative mode) with drift times of 38.5, 39.0, 43.5 and 44.0 ms, respectively, and performed semiquantitative analysis for the differentiation of legal CBD- and illegal THC-marijuana. For forensic purposes, cross-validation with GC-MS and HPLC-UV is currently performed. Future research is aimed at investigating whether the determination of THC, CBD, CBD-acid A and THC-acid A in crude, unextracted plant material is feasible by combination of DART and ion mobility-MS.

Novel aspects: Systematic investigation of the suitability of high-resolution ion mobility-MS for the rapid differentiation of legal and illegal marijuana.

Keywords: tetrahydrocannabinol, cannabidiol, marijuana, ion mobility-MS, forensic chemistry

Rapid Screening of Methylamphetamine in Hair of Drug Addicts using DSA-TOF

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1 Introduction

Quick and accurate detection of methylamphetamine (MAMP) is important for effective control its significant increase of abuse. Comparing to urine specimen testing, hair analysis in forensic has been of great interest for detection of drugs of abuse, because it can provide a longer detection window up to a 90-day drug use history. Normally these measurements are performed using GC/MS or LC/MS, which require extensive and complicated sample preparation.

In this study, a simple preparation and detection method was developed on a Direct Sample Analysis Time of Flight Mass Spectrometer (DSA-TOF MS) system for rapid screening of MAMP abuse in hair. The whole analysis was completed within several minutes. The effectiveness of this method was confirmed by the result of ultra performance liquid chromatography tandem mass spectrometry (UPLC-MS/MS).

2 Experimental

Sample preparation:

After washed with detergent and 0.1% acetone, 50 mg of hair sample was weighed into a glass tube, then 1 mL of 5% NaOH solution (w/w) was added to tube. The tube was put into a water bath (80℃) for 5 minutes, then vortex-mixed for 30 seconds and centrifuged at 6000 rpm for 3 minutes. The final solution was filtered through a 0.2 µm membrane filter. 10 µl sample was loaded onto auto-sampler of DSA. For LC-MSMS analysis, the final solution was diluted for 5 times with water before injection.

DSA-TOF MS Method:

The DSA system was coupled to a PerkinElmer AxION 2 TOF MS equipped with free APCI ionization source operating in positive mode. Mass spectrometer operating conditions were as follows: mass range: 80-1000 Da; APCI Heater Temp: 350 ℃, Auxiliary Gas: 5 psi; Nebulizer Gas: 80 psi; Drying Gas flow rate: 3 L/min; Capillary voltage: 100 v.

Data acquisition and analysis were performed using PerkinElmer TOF MS Driver and EC ID software for identification.

UPLC-MS/MS Method:

A confirmation analysis was conducted using liquid chromatography tandem mass spectrometry. The system included a PerkinElmer Altus™ A-30 UPLC® system coupled to an Ionics 210 triple quadrupole mass spectrometer equipped with an electrospray ionization source operating in positive mode. A PerkinElmer SPP C18 column (2.1*50 mm, 2.7um) was used for separation and the temperature of the column was set at 40 ℃. The mobile phase consisted of water containing 0.1% formic acid (A) and acetonitrile (B). Flow rate was 0.4 mL/min, and the following linear gradient was adopted: 0–2.5 min 10–95% B; 2.5–3.0 min, 95% B; 3.0–3.1 min 95–10% B; 3.1–5 min, 10% B. Injection volume was 2 µL.

Mass spectrometer operating conditions were as follows: ElectroSpray: 5500 v, Heating Gas Temp: 450 ℃, HSID Temp: 320 ℃, Dry Gas: 90, Nebulizer Gas: 180. Detection of analyte by tandem mass spectrometry was conducted in multiple reaction monitoring mode (MRM). 150.0-91.1 and 150.0-119.1 were used for quantitative and qualitative transitions, respectively. Their collision energies were -37 and -14 v, respectively. MRM dwell time was set at 50 ms for each transition.

Data acquisition was performed using PerkinElmer Simplicity 3Q software and quantitation was performed using Simplicity 3Q Quant software.

3 Results

DSA-TOF has been proven to be a good tool for rapid screening of forensic compounds, including MAMP. The analysis of treated samples can be completed within half a minute.

For the sample preparation process, concentration of NaOH, water bath temperature and duration, and different digesting solvents were optimized. A simple but effective extraction of MAMP from hair samples was developed as described in the method session. The rapid analysis combined with high resolution and high mass accuracy is used to unambiguously identify target compounds of drug of abuse in hair samples.

With the optimized method, 10 ppb of MAMP of abuse in hair matrix extract could be detected (Fig 1). This amount translates into measurement of the analyte at 200 pg/mg level from hair, which is lower than the required detection limit (LOD) of drugs of abuse in hair for screening. The precision of the method in LOD level, expressed as RSD, were less than 12.6% (n=5).

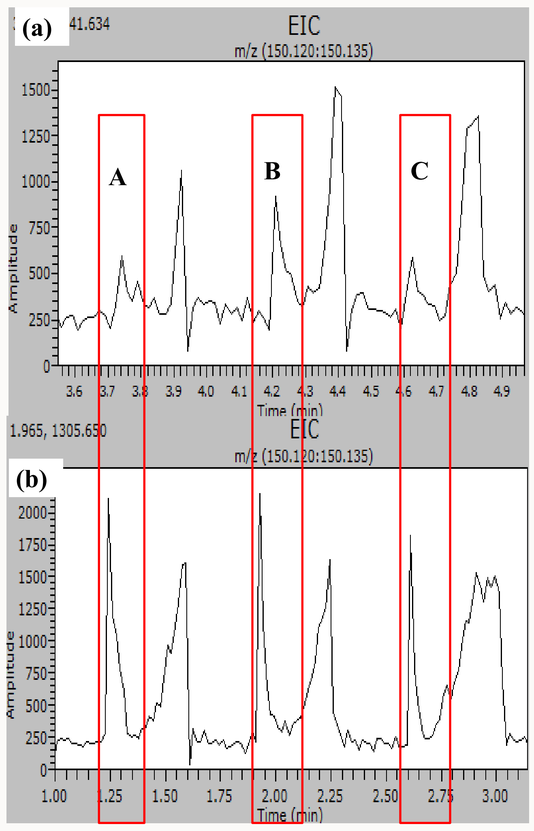

Fig. 1. Typical Extract Ion Chromatograms of hair as acquired by DSA-TOF: (a) blank sample and (b) blank sample spiked with 10 ppb MAMP (EIC window: 150.1277±0.0075 Da)

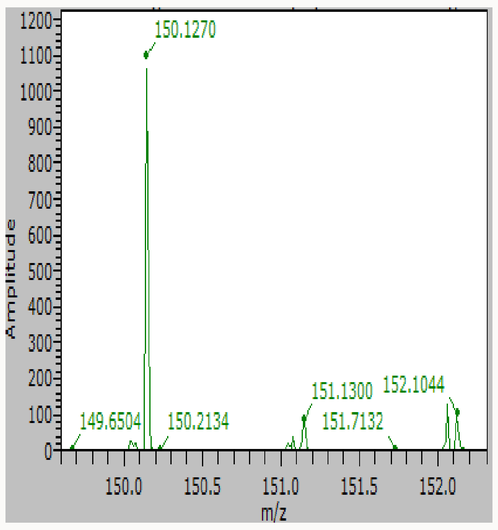

Fig. 2. Typical mass spectra of blank hair sample spiked with 10 ppb MAMP as acquired by DSA-TOF (mass error: 4.7 ppm)

And the mass error of blank hair sample spiked with 10 ppb MAMP as acquired by DSA-TOF below 5 ppm after internal standard calibration and background subtraction.(Fig 2)

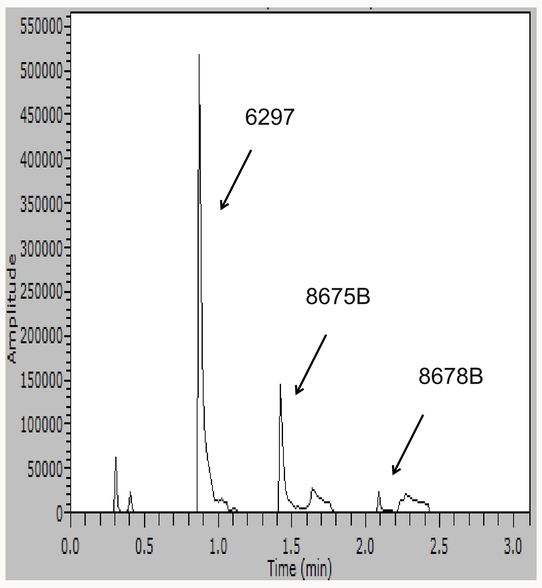

Fig. 3. Typical Extract Ion Chromatograms of real hair sample as acquired by DSA-TOF (EIC window: 150.1277±0.0075 Da)

The developed method was applied to analyze six real samples obtained from suspects. 3 positive residues of the target analyte were found out of the six samples (Fig 3).

LC-MS/MS analysis of the treated samples was performed to validate the above-mentioned results. Method specificity was found to be satisfactory, with no chromatographic interference observed during the retention time of the analyte (Fig. 4).

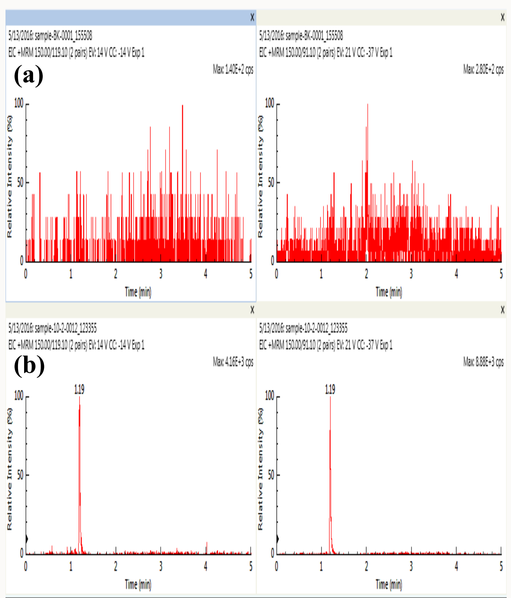

Fig. 4. Typical chromatograms of hair sample as acquired by MRM: (a) blank sample and (b) spiked with 10 ng/ml for MAMP

Response linearity was evaluated by matrix-matched calibration curves, ranged from 1 to 1000 ng/ml for samples. The regression coefficients (r^2) for the calibration curves obtained for MAMP in this study were all above 0.990. The RSD of the method were less than 15% (n=5).

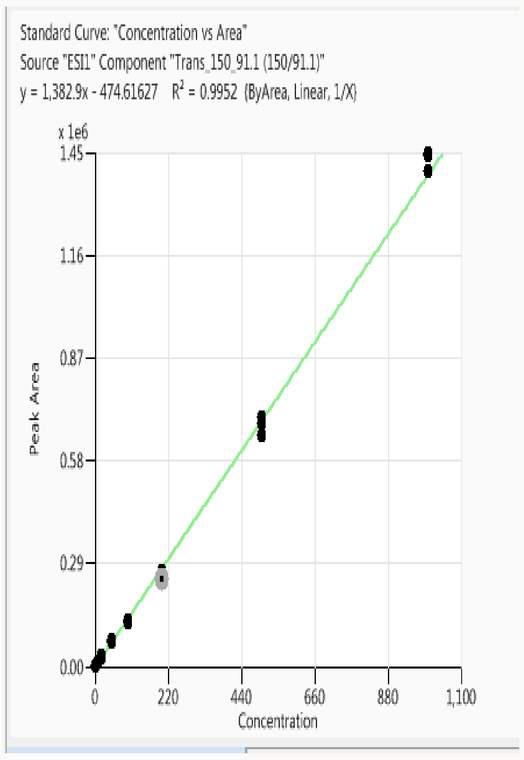

Fig. 5. Typical linearity of matrix-matched calibration curves (n=5)

Results for real sample are 26.5 pg/mg (sample 8678B), 234.0 pg/mg (sample 8675B) , and 998.2 pg/mg (sample 6297), respectively.Typical chromatograms of positive samples are shown in Fig. 6.

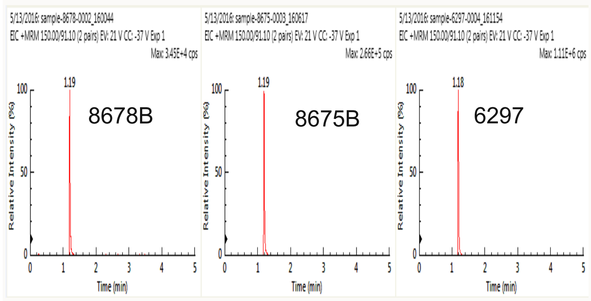

Fig. 6. Typical chromatograms of real sample containing MAMP

References

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4 Conclusions

- In this work, MAMP of abuse at 200 pg/mg level in human hair can be rapidly screened using DSA-TOF. The effectiveness method was further confirmed by LC-MS/MS analysis.
- The optimized method greatly improved the efficiency and is superior to the required detection limit for screening of MAMP of abuse in human hair.

Optimization of the LAMPAS 3 laser mass spectrometer for improved on-line single particle analysis

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Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, Germany

Keywords: mass spectrometry, instrumentation, single particle analysis, delayed ion extraction

INTRODUCTION

Bipolar on-line laser mass spectrometry is a well-proven method to determine chemical and physical properties of aerosol particle ensembles or individual particles. Mobile instruments of this type can be operated directly at sites of interest for *in situ* characterization of aerosols without prior sampling and sample transportation. With such systems aerosol particle characterization is possible with high temporal resolution combined with a high level of specificity. Detailed instrumental characterization and optimization is an essential prerequisite to ensure high-level particle identification during long-term operation of such mass spectrometers.

METHOD

The LAMPAS 3 laser mass spectrometer is a highly robust and compact instrument (Hinz et al., 2011). Aerosol particles are introduced into this instrument using an impact-free inlet system. After particle detection and sizing a pulsed UV laser evaporates and ionizes the detected particles. The generated positively and negatively charged ions are analysed by two time-of-flight mass analyzers. For optimization of the system several instrumental features such as delayed ion extraction, ion reflectors and laser beam attenuation were integrated. Measurements were performed under laboratory conditions with particles of various ambient origins and standard particles such as polystyrene latex spheres, nebulized salt solution particles and mineral particles for characterization of the instrumental performance.

RESULTS

For detailed investigation of mass resolution of ion signals hundreds of spectra detected from particles generated by nebulization of salt solutions were evaluated for various delay times after ion generation. Such measurements were performed for two different conditions in the ion source region of the mass spectrometer. For these experiments the field strengths in this region was varied. As a result it was found that for isotops of iron and lead in the positive ion mode an improvement of mass resolution by a factor of 1.5 is possible. The delay times for ion extraction vary with electrical field strength. The stronger the electrical field the shorter the delay time has to be, because small differences in position of two ions

have high influence on ion acceleration when applying the electrical field. The described instrumental improvements and optimization of LAMPAS 3 resulted in an analytical system for advanced *in situ* particle characterization and identification under various conditions and requirements.

References

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Novel aspects

Improvement of mass resolution in single particle analysis by delayed ion extraction

Tandem Mass Spectrometry with a (Ultra-)High Resolving Time-of-Flight Mass Spectrometer

Julian Bergmann[1], Wayne Lippert[1], Johannes Lang[1], Timo Dickel[1,2], Wolfgang R. Plaß[1,2], Hans Geissel[1,2], Christoph Scheidenberger[1,2], Mikhail Yavor[3], Alexander Pikhtelev[4], Samuel Ayet San Andrés[1,2]

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Introduction

Common compact mass spectrometers are typically limited to low or medium mass resolving power. In order to overcome this limitation, a mobile multiple-reflection time-of-flight mass spectrometer (MR-TOF-MS) has been developed that allows for sub-ppm accuracy with (ultra-)high mass resolving power in a compact size [1,2]. It is capable of resolving isobars and determining the structure and composition of molecules for in-situ measurements [3].
Furthermore the device offers multiple-stage tandem mass spectrometry with very high mass resolving power in every stage using the novel technique of mass-selective ion-trapping.

Experimental

The setup, mounted inside a single frame of 0.8 m^3, consists of an atmospheric pressure inlet for various ion sources, a beam preparation system (RFQ ion guide, mass filter, cooler and trap) a time-of-flight analyzer with a mass range selector and a detector [2]. For MS/MS experiments , after the ions are dispersed in time-of-flight according to their mass-to-charge ratios, they are re-trapped in the original injection trap with high mass separation power [4]. There they are fragmented using CID before their fragments are measured with (ultra-)high resolving power [3]. A software package was designed and developed for hardware control, data acquisition and for online and offline analysis.

Results and Discussions.

The mobile MR-TOF-MS can reach mass resolving power up to 300 000 with flight times over 17 ms. In MS/MS applications mass separation power of over 70 000 after 3.6 ms flight time and re-trapping efficiencies of up to 35% has been reached for precursor selection of caffeine molecules. Glutamine and Lysine were successfully isolated from their respective isobaric contaminants within 0.23 ms and their isolated dissociation spectra have been measured [3].
Since the device allows for tandem-in-time, there is no general limitation on the number of separation steps. To illustrate this MS^3 of lysine was performed and measurements of the isolated fragments taken in all steps.

New Aspects

MS/MS precursor selection with separation power 70 000 in a compact mass spectrometer; MS^3 in a TOF-MS.

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[4] T. Dickel et al., *Retrapping*, submitted, JASMS (2016)

Keywords:
tandem mass spectrometry, time of flight, high resolving power, high separation power

Topics:
Instrumentelle Entwicklungen

Field ionization: an old but still useful method

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one of the major tasks in mass spectroscopy is the determination of the molecular weight. In LCMS there are various methods for soft ionisation on the market. In GCMS electron impact ionisation dominate the field as a fast identification by databasing is possible. However for the determination of molecular weights EI is not very effective

Experimenteller Teil

We compared the EI, methane CI , ammonia CI and the FI spectra of various compounds. with respect of molecular weight determinations.

Ergebnisse und Diskussion

For most of the compounds EI and CI will lead easily to the molecular weight information, but there are still some compounds where we found FI to be much easier to get this information .

the major limitation of FI is the low sensitivity compared to the other method, so that it is not usefull for trace analytics.

Neue Aspekte

we found FI is still a valuable tool to determine the molecular weight in GCMS

Rapid On Site Analysis of BTX with Portable GC/MS

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BTEX aromatics (benzene, toluene, ethylbenzene and xylenes) are frequently encountered environmental pollutants. A miniaturized GC/MS (weighing 14.5 kg, complete with battery and carrier gas) is utilized to rapidly survey air, water, and soil samples on site for the presence of these compounds.

Experimenteller Teil

Volatile organic compounds are introduced into the GC/MS with either of two sampling methods. The first sampling method is Solid Phase Microfiber Extraction (SPME) and the second sampling method is Thermal Desorption (TD).

Ergebnisse und Diskussion

It is possible to get within shortest time (10 - 15 min) results to make timely decisions and to solve problems.

Neue Aspekte

The possibility to make on site decisions about environmental contaminations.

Multiple analysis of individual airborne aerosol particles by on-line laser mass spectrometry: Detection of polyaromatic hydrocarbons from the particle-surface and inorganic constituents from the particle-core

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[2]*Joint Mass Spectrometry Centre Helmholtz-Zentrum München, Comprehensive Molecular Analytics (CMA), Neuherberg, Germany*

Introduction

Single particle aerosol mass spectrometry (MS) became a versatile method for characterisation of ambient airborne particles. Available systems are based on laser desorption/ionization (LDI) in the ion source of an Aerosol Time-of-Flight MS (ATOF). Particle LDI is typically restricted to detection of inorganic compounds or fragments. However, a better understanding of particle bound organic compounds is of particular interest. For the health-relevant polycyclic aromatic hydrocarbons (PAHs), a single-particle approach was developed [1]. Herein, PAHs are desorbed by an IR-laser pulse before being ionized by an UV-laser pulse via resonance enhanced multiphoton ionization (REMPI). The drawback is that the normal LDI-information on the inorganic bulk composition cannot be retrieved and classification of the particle core (for source apportionment) is not possible.

Experimental

We present a new method for the detection of a) intact PAHs by REMPI and b) elemental ions from the core (LDI) of the same, individual aerosol particle: Firstly, airborne particles are introduced and sized by laser velocimetry. Closed to the ion source, an IR-laser pulse hits the particle for desorption. PAHs from the plume are now (REMPI-) ionized by a following UV-pulse and accelerated into the dual TOF-analyzer. After extraction, the ion-source field is reversed. Now, a third pulse (ArF-excimer, 193nm) hits the residual core for LDI. Due to field-inversion, LDI-cations are accelerated into the opposite TOF-analyzer. By this procedure, the REMPI-spectrum and the LDI-spectrum of inorganics from the same individual particle of known size are detected.

Results & Discussion

The new system was set-up, optimized and tested. It was shown that individual particles could analysed sequentially according to their organic and inorganic content by the new single particle aerosol mass spectrometer. The first application measurements were performed with re-dispersed combustion particles, namely coniferous wood combustion- and diesel exhaust-particles. The two particle types show specific peak signatures for the organic adsorbat layers as well as for the inorganic particle cores. Alkylated phenanthrenes, in particular retene (234 m/z, shell, REMPI) as well as K^+ and Na^+ (core, LDI) are detected for wood combustion particles. Diesel particles show non-alkylated PAHs (shell, REMPI) and C^+ or Fe^+ (core, LDI). The C^+-peak as well as higher carbon clusters (C_2^+, C_3^+ etc.) indicate the carbonaceous character (soot) of the particle core. Furthermore it could be shown that soot-type particle-cores are more often associated with PAH-signals (shell) than inorganic particle-cores. Thus the new on-line multi-step laser photo-ionization single particle mass spectrometry approach represents a promising technology for source apportionment as well as the analysis of internal and external mixings state of the different chemical particle constituents.

References

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Keywords: Single particle aerosol mass spectrometry, ATOFMS, laser desorption–laser post ionization, LDI polycyclic aromatic hydrocarbons, inorganic core

Category

Instrumental development

Ionisation techniques

Titel:

Thermogravimetry coupled to Ultrafast Gas Chromatography Singlephoton-Ionisation Time-of-Flight-Mass-Spectrometry (TG-SPI-TOF-MS) for Evolved-Gas-Analysis of Fuels regarding to the Deposit Formation Potential

Authors:

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Introduction

Throughout the combustion of fuels in combustion chambers deposits can be formed as a result of incomplete burning, hot spots and less supply of oxygen. With the increased addition of biofuels to reduce emissions changes in fuel pattern and behaviour under thermal stress will occur. Depending on the quality and biofuel content the fuels show a different deposit formation potential but it is difficult to assign responsible molecular species [1,2]. Using a particular fingerprint can point out details about the formation mechanism. The knowledge about organic content in deposits is actually limited, especially during the combustion process [3]. With the coupling of Thermal Analysis to a selective and high separating Mass Spectrometer the organic compounds can be analysed temperature-dependent [4].

Experimental

For a well described fingerprint of complex samples a selective, not destructive method with a high separation power should be used. The coupling of a thermobalance STA 449 Jupiter (Netzsch Gerätebau GmbH, Selb, Germany) to a Photoionisation Time-of-Flight Mass Spectrometer (Tofwerk AG, Thun, Switzerland and Photonion GmbH, Schwerin, Germany) for a soft photoionisation with one photon at 116 nm (Single Photon Ionisation, SPI) can fulfil this qualifications. The sample will be heated up by 10 K/min in a small alumina pan under nitrogen atmosphere meanwhile recording the mass loss. To improve the separation process of evolved gas phase compounds an additional ultrafast GC step of 60 s with temperatures from 90 up to 320 °C can be connected [5].

Results

The first separation step can be achieved by the evaporation using a thermobalance, which can record the mass loss during the heating procedure. The second dimension results by a fast GC separation step, which allows to differentiate between signals of isomers with similar boiling points like Nonane and Naphthalene in less than 60 s. Finally with the soft ionisation the mass spectra with nearly no fragmentation products for high molecular compounds represent the third dimension. A comparison of two low-sulphur heating oils point out nearly the same thermal properties as heating and calorific value, density or distillation curve. Contrary the fingerprints of these two oils show differences in higher molecular level as Polycyclic Aromatic Hydrocarbon (PAH) composition. Especially at temperatures in the area of pyrolysis the mass loss for one heating oil reveals higher thermal fragmentation processes and belonging mass spectra show less PAH distribution.

Interestingly the heating oil which is subject to increased thermal fragmentation tend to a smaller deposit formation potential and evaporation residues, whereas the heating oil with higher PAH content and resistance to thermal degradation form more than twice the amount of deposits.

New Aspects

The hyphenation of ultrafast GC-SPI-TOFMS for evolved gas analysis to a thermobalance allow the detailed fingerprinting of fuels and deposits.

Keywords

Photoionisation, Fuel Characterisation, Thermal Analysis

Category

Instrumentelle Entwicklung, Ionisationsmethoden

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Single-photon ionization of laser desorbed molecules in a fine-vacuum ion source

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Single-photon ionization (SPI) is a relatively 'soft' method for generating molecular ions from a broad chemical range of small molecules, including non-polar compounds. SPI has been coupled with e.g. laser-based desorption using high-vacuum ion sources [1]. In the more established atmospheric pressure photoionization (APPI), the ionization is typically supported by usage of dopants which are ionized in SPI processes and transfer their charges to neutral analytes via secondary pathways [2].

Here we present the first example of adapting a low-cost Kr-VUV-lamp to a laser desorption/ionization source operated at ~1 mbar of N_2 and optional use of nebulized dopants. We show that this postionization approach has a high potential for boosting the ion yields for several classes of laser-desorbed molecules.

Experimenteller Teil

The Kr-VUV lamp (PKS106, Heraeus, emission at 117/124 nm) was integrated into an oMALDI2 ion source (AB Sciex).The source was mounted to a QSTAR *pulsar-i* mass spectrometer (AB Sciex) and operated with variable buffer gas pressure (N_2) between 0.1-1.0 mbar [3]. A capillary was used to optionally introduce dopant gas (acetone). The total pressure in the source was monitored by a gas-independent pressure gauge. Physiologically important lipophilic biomolecules that are difficult to ionize by standard MALDI were selected as test samples. These were either spotted onto *Drosophila melanogaster* fly wings for matrix-free surface-assisted laser desorption/ionization (SALDI-)MS [3] or, in some cases, embedded into a 2,5-dihydroxybenzoic acid (DHB) MALDI matrix. Desorption was achieved with an N_2 laser (337 nm).

Ergebnisse und Diskussion

In agreement with our previous studies [3, 4], SALDI-MS utilizing fly wing substrates produced molecular $[M+Na]^+$ and $[M+K]^+$ ions of many simple (such as unsaturated hydrocarbons) as well as more complex lipids (such as free fatty acids, triacylglycerols, or β-carotene). However, the signal intensities for certain other physiologically relevant hydrophobic analytes, such as cholesterol, were only low.

Engaging the VUV lamp and introducing acetone as a dopant increased the cholesterol signals by more than one order of magnitude: a strong $[M-H_2O+H]^+$ ion signal was now obtained, next to low intensity signals of $M^{+\bullet}$, $[M+H]^+$, and $[M-H_2O]^{+\bullet}$ species. For other, e.g., also the SALDI-detectable lipids, a notable shift in the ion patterns was observed: in several cases (such as for β-carotene) $M^{+\bullet}$ and $[M+H]^+$ ion species were dominating the SPI-based mass spectra. This feature could be exceedingly helpful for tandem MS measurements. For triolein, high abundances of additional $[M+H]^+$ signals and those corresponding to neutral loss of one C18:1 residue (FA) to $[M-FA+H]^+$ were detected. In a MALDI experiment, strong $M^{+\bullet}$ signals of the polycyclic aromatic hydrocarbon naphthalene were produced only when the Kr-lamp was in use.

Besides for the dopant, the buffer gas pressure in the ion source was found to have a strong effect on the monitored ion yields. For example, in comparison to an in-source pressure of 0.7 mbar of N_2, a six-fold increase of the cholesterol signal was obtained at 0.4 mbar. This finding might be explained by the plume expansion dynamics resulting in optimal overlapping between particles, dopant, and VUV photons in the assembled prototype ion source. Based on the obtained promising results – and following further optimization of the geometries - this low-cost postionization approach could offer a large potential for widening the application range of comprehensive laser-based mass spectrometry.

Neue Aspekte

First report on successful dopant-assisted VUV single-photon ionization of numerous lipid classes in a fine-vacuum LDI ion source.

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Full Characterization of Antibodies Under Denaturing and Native Conditions on a Hybrid Quadrupole-Orbitrap MS Equipped With a Higher Mass Range

Kai Scheffler, Eugen Damoc, Tabiwang Arrey, Martin Zeller, Jennifer Sutton, Aaron Bailey, and Jonathan Josephs

Introduction

MS analysis of antibodies at the protein and peptide levels is critical during development and production of biopharmaceuticals. The compositions of current generation therapeutic proteins are often complex due to various modifications which may affect efficacy. Intact proteins analyzed by MS are detected in higher charge states that also provide more complexity in mass spectra. Protein analysis in native or native-like conditions with zero or minimal organic solvent and neutral or weakly acidic pH decreases charge state value resulting in mAb detection at higher m/z ranges with more spatial resolution.

Experimental

Three commercially available monoclonal antibodies were used for all experiments. Intact proteins were desalted online using size exclusion chromatography (SEC) or reversed phase chromatography coupled on-line with a mass spectrometer.
For peptide analysis antibodies were proteolytically digested with and without prior reduction and alkylation. The mass spectrometer used for all experiments was a commercially available hybrid quadrupole-Orbitrap mass spectrometer equipped with the new BioPharma option providing capabilities to allow for improved high mass transmission and mass detection up to 8000 m/z.

Results and discussion

We have analyzed the profiles of three monoclonal antibodies under reducing and native conditions by direct infusion with offline desalting and with on-line desalting via size exclusion and reversed phase type columns. The presence of high salt under denaturing conditions was found to influence the observed charge state envelope and impacts mass accuracy after spectra deconvolution. The significantly lower charge states observed under native conditions improves the spatial resolution of proteins signals and has significant benefits for the analysis of antibody mixtures, e.g. observed as lysine variants, degradations or sequence variants. This type of analysis requires the detection of masses beyond the standard mass range ranging up to 6000 m/z requiring the extended capabilities allowing mass detection up 8000 m/z.

We have compared each intact antibody sample that was analyzed individually with mixtures in various relative concentrations. For analyses on the peptide level we analyzed reduced/alkylated and non-

reduced proteolytic digests of the individual antibodies separated via reversed phase chromatography aiming to retrieve as much information as possible regarding sequence coverage, disulfide bridges, post-translational modifications such as various glycans, sequence variants and their relative quantification. All data acquired were submitted to a single software package for analysis aiming to obtain a complete picture of the molecules analyzed. Here we demonstrate the capabilities of the mass spectrometer to fully characterize homogeneous and heterogeneous therapeutic proteins on one single platform.

Novel aspect

Three major workflows for characterization of biopharmaceuticals on one single LC-MS platform using single and mixed antibody samples are presented.

LIPIDOMICS QUANTITATION USING A NOVEL SCANNING QUADRUPOLE DIA METHOD

Chris Hughes, Keith Richardson, Jason Wildgoose, Lee Gethings, James Langridge, Mike Morris and Johannes PC Vissers
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INTRODUCTION

Targeted LC-MS based assays are increasingly applied in the post-discovery omics area with emphasis on validation, the first of many phases in translational analyses, or in studies that are aimed at gaining the understanding of biological systems, drug development and treatment. Context is driving current omics experiments, thereby driving the development of LC-MS acquisition methods that can provide both qualitative and quantitative information in a single experiment. A novel Data Independent Acquisition technique - SONARTM - that satisfies both these requirements, will be demonstrated.

In the method, a low-resolution quadrupole mass filter is scanned repetitively and both precursor and MS-MS data acquired at spectral rates approaching 2000 spectra/s. The method produces a high duty-cycle, highly specific and unbiased two-dimensional data that can be viewed and processed using readily available informatics. The mode of operation has been implemented on a bench top quadrupole - ToF mass spectrometer and has been applied to targeted lipidomics experiments involving the quantitation of lipids in human plasma samples derived from normal, obese and diabetic donor cohorts.

METHODS

Sample preparation

Standards. A pre-mixed synthetic lipid standard mixture (Avanti Polar Lipids, Inc.) served as a lipidomics standard that was serially diluted in a human plasma extract.

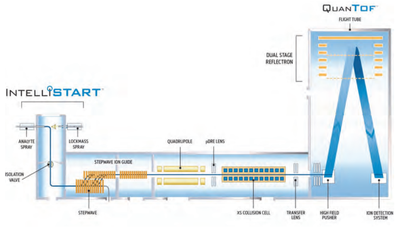
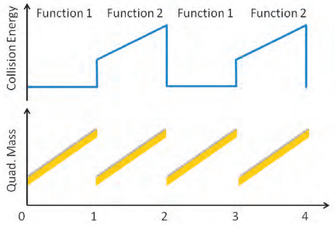


Figure 1. Xevo G2-XS QTof Mass Spectrometer instrument schematic.

Biological samples. Lipids were extracted from human plasma (Innovative Research Inc), which originated from 6 control, 6 obese and 6 diabetic patients. Lipid extractions were performed as previously described1. The extracts were centrifuged for phase separation and the lower fraction collected for LC-MS analysis.



Expt	Ion Mode	Quad Scan (Da)	Quad Window (Da)	ToF Scan (Da)	Function Integration Time (s)	Fn 1 CE (V)	Fn 2 CE (V)
Lipidomics	+	500 to 1200	10	50 to 1000	0.1	6	20 to 50
Lipidomics	-	500 to 1200	10	50 to 1000	0.1	6	25 to 55

Figure 2. SONARTM acquisition method and DIA acquisition parameters used.

LC-MS conditions

The LC-MS experiments consisted of a 20 min gradient from 3 to 40% isopropanol:methanol (10 mM ammonium formate) at 500 µL/min using a ACQUITY LC system. Here, a BEH 1.7 µm C8 reversed phase 2.1 x 10 cm LC column was used.

A Xevo G2-XS QToF (Waters Corporation), Figure 1, was operated in SONARTM 2DMS mode. The optimized quadrupole window and the other parameters employed for lipid analyses are described in Figure 2.

Bioinformatics

SONARTM DIA data were processed with UNIFI (Waters Corporation) or Progeneseis QI (Nonlinear Dynamics) using optimized threshold and compound search parameters. Quantitative analysis was performed with Skyline (University of Washington) using fragment elemental composition derived from Progeneseis QI MS/MS libraries.

RESULTS

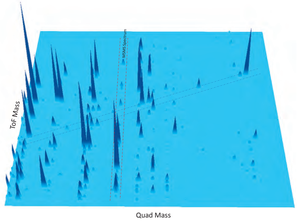


Figure 3. SONARTM DIA ToF vs. quadrupole m/z data, showing product ions (vertical bands) from peptides eluting over a 1 min window and the quadrupole sweep (diagonal line).

Specificity

Figure 3 represents typical omics SONARTM data and demonstrates that the data format is the same as other multi dimensional datasets, eg ion mobility; hence, exhibits improved specificity. When viewing these data, the drift time axis is replaced by quadrupole mass.

Concept

Shown in Figure 4 is the conceptual use of the SONARTM 2DMS DIA data whereby precursor and product ions are extracted in multiple dimensions, i.e. retention time and first (quadrupole) and second (ToF) mass analyser m/z. The following sections will demonstrate that this data can be utilized for both qualitative and quantitative analysis of lipidodomics data.

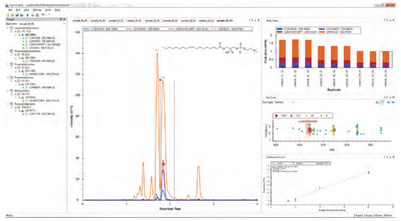


Figure 4. Multiple dimension ion extraction using retention time, quadrupole (precursor) m/z and ToF (product ion) m/z for a synthetic lipid mixture spiked into human plasma extract.

Discovery lipidomics

The ability to search and quantify (relatively) SONARTM DIA lipidomics data is shown in Figure 5, highlighting disease specific lipid compounds.

Figure 5. Discovery lipidomics DIA 2DMS analysis illustrating identification, compound distribution, and grouped lipid quantitation/hierarchical clustering.

Targeted lipidomics

A number of analytes were selected for targeted analysis of the data, Figure 6. Precursor/product ions list were provided to the software, along with quadrupole (precursor) *m/z* extraction information. Both examples show the presence of specific and a-specific product ions which can be readily identified and discarded for further down-stream quantitative analysis.

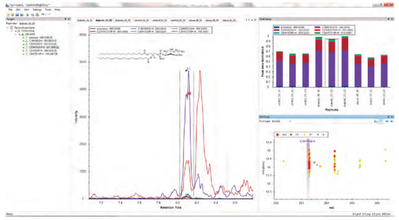
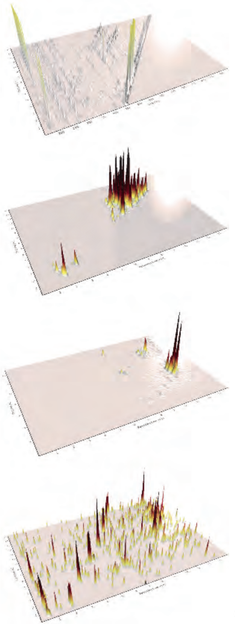


Figure 6. Targeted analysis of potential/reported disease specific lipid (phosphatidylinositol) markers of interest related to either obesity or diabetes.

Class analysis

Class specific information can be readily extracted from the multidimensional data as shown by the mass extracted multi-dimensional product ion maps in Figure 7, representing lipids that are typical for the studies samples.



(A) product ion m/z range

(B) m/z 184 (PCs)

(C) m/z 264 (Ceramides)

(D) m/z 225 (PAs)

Figure 7. Class specific SONARTM DIA product ion maps for (A) all lipids, (B) phosphocholines (PC), (C) ceramides, and (D) phosphatidic acids (PA).

Application results validation

Application of SONARTM to discovery omic studies investigating obesity and diabetes has identified key targets including a variety of lipid classes involved in metabolic syndrome related pathways as shown in Figure 8. Quantitative profiles observed for a subset of the detected phospholipids map to the phagocytosis pathway and correspond with previous findings linking B1 B cell phagocytosis with high fat diets[2].

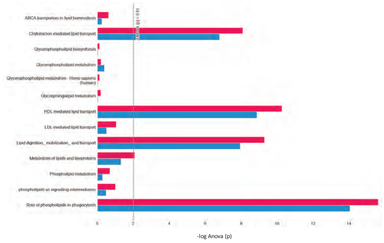


Figure 8. Combined pathway analysis of lipid and protein datasets using IMPaLA (proteomics data not shown). Statistically relevant lipids (blue) and proteins (pink) above a threshold of 0.01 ANOVA (p) are considered (e.g. HDL mediated transport[6] and chylomicron-mediated transport)

CONCLUSION

- **Novel, data independent acquisition mode of acquisition with high duty cycle and precursor ion specificity for the application of lipid analysis.**
- **SONARTM DIA acquisition provides multi dimensional data sets exhibiting improved specificity and over other DIA methods**
- **SONARTM data acquired in lipidomics experiments shows excellent qualitative and quantitative characteristics and can be applied in discovery, targeted and translational lipidomics studies**
- **Application of SONARTM detected and quantitatively confirmed known diabetes/obesity lipid indicators**

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Thermal and laser desorption atmospheric pressure photo ionisation ultra high resolution mass spectrometry – Concept and application towards complex samples

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Introduction

Evolved gas analysis (EGA) coupled to high resolution Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) is a powerful tool for analysing complex samples such as fossil fuels and their derived combustion aerosols on molecular level. [1]

Sample introduction before ionisation is a key parameter in mass spectrometry. For EGA, thermal desorption (TD) is often utilized. Nonetheless, various desorption techniques such as DESI and LDI exist [2]. Separating laser desorption (LD) and ionisation reveals certain benefits such as the application of lower energy densities for preventing artefacts.

After introduction, atmospheric pressure photo ionisation (APPI) is a suitable ionisation method due to its capability to ionize a broader chemical space in contrast to other API techniques such as APCI or ESI [3].

Experimental

TD-APPI was realized via a homebuilt desorption unit equipped with a 100 W heating cartridge and a krypton lamp (10.6 eV) respectively a xenon lamp (9.6 eV) for ionization. Samples were measured with a defined heating rate of 10 K/min up to 350 °C.

Besides TD, LD was realized utilizing a 3 W laser diode with a lens which focusses the beam to a diameter of approximately 2 mm. For evaluation, the pulse length of LD, energy and focus were varied. Critical aspects are desorption without changing the sample and the plume concertation.

Mass spectra were acquired with a mass resolution of R=300 000 @400 m/z utilizing a Solarix FT-ICR MS (Bruker, Germany) equipped with a 7°T superconducting magnet.

Results and Discussion

The setup, both thermal desorption and laser desorption, was evaluated with standard substances and standard mixtures. For the approach towards complex mixtures, several

petroleum samples such as diesel fuel, marine gas oil, and heavy fuel oil as well as their derived combustion aerosols were analysed.

The ionisation with APPI produces mainly protonated molecular ion species for components of complex mixtures which could be formed through proton transfer reactions.

TD shows a simulated distillation-like behaviour for the mixture`s compounds which means that the average mass over charge ratio was shifted to higher values for higher temperatures (up to m/z 600) and is therefore capable for analysing volatile and semi-volatile components. Especially for combustion aerosol samples, 350 °C are not sufficient for evaporating all organics adsorbed on the particulate matter. However, it could be shown that LD exhibits species with higher m/z. Particularly for the investigation of heavy petroleum fractions, the higher end of the distribution is accessible, which is not feasible with the thermal desorption. Nonetheless, thermal desorption can be seen as a type of separation, lowering the complexity of mixture in the atmospheric pressure source to prevent matrix effects and revealing details about the release profile (which could be addressed to structural aspects or stability).

Summarizing, both techniques have different advantages for the analysis of complex samples and can be used complementary as well as combination for addressing first the volatile and semi—volatile compounds with TD—APPI and second the heavier species with LD-APPI.

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New aspects

Versatile ionisation source enabling thermal and laser desorption for investigation of complex and high boiling point materials via FT-ICR MS.

Topics

Instrumentelle Entwicklungen
Umweltanalytik

Keywords

high resolution mass spectrometry, evolved gas analysis, atmospheric pressure ionisation, thermal desorption, laser desorptio

Quantitation of Proteomics Samples Using a Novel Scanning Quadrupole DIA Method

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Targeted LC-MS assays are increasingly applied in the post-discovery proteomics area with an emphasis on validation. A novel DIA mode of operation, which provides both qualitative and quantitative information, has been developed for a tandem quadrupole/oa-time-of-flight (ToF) MS and applied to targeted proteomics experiments using transition extraction lists and compound library based approaches.

Experimenteller Teil

NanoLC was performed with a Waters Nanoacquity UPLC equipped with a 75micron x 150mm column. The *m/z* isolation range of the quadrupole was continuously scanned with MS data acquired up to a frequency of 400 spectra/s. Alternate MS scans comprised precursor and CID product ions. The resulting 2D data, *m/z* (ToF) *vs. m/z* (quadrupole) were processed using Progenesis QIP and Skyline informatics.

Ergebnisse und Diskussion

Quantitative proof-of-principle data were acquired by serially diluting a four protein digest mixture into a proteolytic *E.coli* digest and quantitative information obtained by using transition extraction lists. Analysis of the data indicates that scanning quad DIA enables over an order of magnitude more specificity than a static quad operated with the same resolution and it was found that a quadrupole transmission window of approx 20 - 30 Da provided optimum protein identifications.

Aliquots of control, diabetic and obese human plasma samples were digested with trypsin overnight. 2DMS data were collected and differentially expressed peptides and hence proteins across the three conditions were quantified. Results show that peptides from apolipoproteins exhibited the most significant changes in good agreement with expected changes in relation to disease and/or phenotype.

Neue Aspekte

Targeted quantitation in proteomics using a novel precursor quadrupole scanning based DIA method

Improving the performance of the airborne laser-spark ion source for the detection of volatile organic compounds under ambient conditions

Andreas Bierstedt, Jens Riedel

Einleitung

Recently, a novel ionization scheme for ambient mass spectrometry has been introduced.[1] Desorption and ionization are achieved by a quasi-continuous laser induced plasma (LIP) ignited in front of the atmospheric pressure interface of a time-of-flight mass spectrometer. This setup comprises the advantages of *i*) an ambient probe, *ii*) electro neutrality, *iii*) low power consumption, *iv)* a sufficient duty cycle, *v*) a ubiquitous plasma medium (air) and *vi*) high sensitivity caused by the high electron number densities.

To assess its future applicability for the detection of gas-phase analytes, plasma properties and operating conditions are investigated to understand the processes, that lead to the formation of molecular ions. Comprehensive studies include optical emission spectroscopy, shadowgraphic shockwave visualization and time-of-flight mass spectrometry investigations.

Experiment

The LIP is ignited directly in the open lab environment in front of a modified atmospheric pressure interface of an orthogonal time-of-flight mass spectrometer by focusing the second harmonic of a high repetition rate DPSS laser (λ = 532 nm, 26 kHz) through an aspherical lens (f = 8mm, N_A = 0.50).

For the gaseous sample introduction an adjustable carrier gas was fed through a temperature controlled liquid sample reservoir. The resulting enriched gas stream was then introduced to a capillary that is placed in line with the LIP and the MS inlet.

Emission spectroscopy and shadowgraphy imaging revealed insight into the physical and chemical plasma properties.

Ergebnisse

The observed MS signal (including reagent-ion signal, as well as analyte spectra) closely resembles the ionization behavior of other electrically-driven plasma-based ionization sources, such as DBD, LTP or DART. This means that although LIPs are commonly known to have temperatures far above 10.000 K and thus efficiently atomize molecules and subsequently form elemental ions, MS spectra were obtained that showed the formation of intact molecular ions.

For an insight into the LIP properties the optical emission of the LIP is examined and exhibits a pronounced degree of dissociation into atomic and ionic species, which reflects the higher temperature and electron density inside a LIP. Accordingly, rather elemental (like in the case of ICP) than molecular spectra should be expected. However, due to the absence of such ions, we conclude that the analyte does not enter the hot center of the plasma itself. Moreover, the initial, highly-excited plasma species react cascade-like to form lower energetic species via reactive collisions with the surrounding atmosphere, which can then eventually ionize the molecules of interest. The concept potentially involves charge transfer, proton transfer, electron impact and photoionization.

These assumptions are confirmed by the shadowgraphs of the expanding shockwave around the LIP. An effective spatial separation between the two regions is maintained by concentrically expanding pressure waves resulting in a strongly unidirectional diffusion. Additionally, the strictly outbound matter transport suggests a rarefaction inside the plasma region for each plasma event. This effect can be compensated by the application of a gas stream to support the diffusive transport into the former plasma zone.

Such an active gas replenishing is found to result in a strong increase in emission brightness, in local reactive species concentration around the LIP, and eventually in direct mass spectrometric sensitivity. As carrier gas compressed air, nitrogen, argon and helium were tested.

Literatur

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High resolution trapped ion mobility mass spectrometry analysis of isomeric compounds

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In combination with mass spectrometry, the use of ion mobility separation opens another dimension for the identification and characterization of known and unknown compounds. It permits to separate isobaric compounds according to their respective collision cross sections. Depending on the type of sample introduction, ion mobility separation can be used for direct infusion experiments as well as for LC-MS analyses of complex samples. Here we describe the separation of various isomeric compounds to facilitate their mass spectrometric characterization. The examples used were isobaric trisaccharides or lipids, which are otherwise difficult to analyze.

Experimenteller Teil

Mixtures of isomeric analytes of different structural classes were prepared from the pure standard compounds. In direct infusion experiments, the TIMS device was used to resolve the isobaric compounds. Therefore, the ions were trapped in a first step. Subsequently, ramped electric field gradients were used to release the ions according to their mobility in a constant gas flow. The TIMS device was tuned for a maximum resolving power to separate the isomers. The MS and MS/MS spectra of compounds were investigated considering mass accuracy, the true isotopic patterns and the fragmentation behavior.

Ergebnisse und Diskussion

Several mixtures of isomeric compounds of different structural classes were investigated, such as. Several of the isomeric compounds showed very similar or identical retention times in standard screening LC-gradients. This complicated the interpretation of MS and MS/MS spectra in standard analyses. In the case of lipid analysis, the interpretation of fragment spectra is further hampered by partially overlapping isotopic patterns of lipids with one additional or fewer double bond. Here, the additional dimension of ion mobility helped to obtain clean MS and MS/MS spectra for compound characterization. All isobaric compounds could be baseline separated in the mobility domain. The respective resolving powers are reported. From the $1/k_0$ mobility values, the collision cross section (CCS) values were calculated and compared to data found in literature. The QTOF data delivered exact masses in the ppm range as well as true isotopic patterns of MS and MSMS spectra. The fragment spectra after mobility separation were evaluated as well as the isotopic pattern qualities. For lipid analysis the mobility separation simplified the identification due to clean isotopic patterns of fragment peaks. The value added by the additional ion mobility separation for the identification of unknown analytes was demonstrated to be enormous.

Neue Aspekte

Investigation of the use of HR trapped ion mobility MS to identify isomeric lipids and trisaccharides by pure MS/MS analysis.

The Usage of Direct Inlet Probe in combination with High Resolution Mass Spectrometry

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The direct probe technique is a well established, fast and convenient method to analyze solid and liquid samples using mass spectrometry. This supplement was coupled to a GC-High Resolution TOFMS with a mass resolution of 50,000 FWHM and mass accuracies less than 1 ppm. The system can be used in GC-MS mode with chromatographic separation or for the direct analysis of solid and liquid samples. Applications, as molecular weight determination and screening methods, are highly applicable for this hardware combination.

Experimenteller Teil

The DIP system enables direct analysis of liquid and solid samples, which need no preceeding chromatographic separation. The results are an enhancement of the GC-HighRes TOFMS application range and faster analysis times. A push rod is used to insert the sample into the vacuum of the ion source to record the mass spectrum. The tip of the push rod keeps the inlay with the sample. The sample is transferred into the vacuum of the ionization chamber via a specially designed vacuum-lock-assembly. When the push rod is fully injected, the probe tip is heated. The analysis were performed in EI mode using a LECO Pegasus® GC-HRT (mass resolution of up to 50,000 FWHM and mass accuracies less than 1 ppm).

Ergebnisse und Diskussion

The combination of DIP/HighRes TOFMS is ideal for the analysis of solid and liquid samples in numerous application areas, such as general chemistry, material science,natural products, pharmaceuticals,metabolomics, food and environmental analysis. It also allows fast screening of quality identification of unknown analytes.The instrument's high resolving power in combination with its excellent mass accuracy values results in confident formula determination. In addition, complete and high quality spectra facilitated library.

Neue Aspekte

Direct inlet probe supplement for a GC-TOFMS system, using folded flight path technology

IR-MALDI Ion Mobility Spectrometry: Low and High Field Mobilities of Peptide Ions at Intermediate Pressure

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3 BAM Federal Institute for Materials Research and Testing, Richard-Willstätter-Straße 11, 12489 Berlin
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Einleitung (max. 120 Wörter)

In ion mobility (IM) spectrometry, ions are separated according to their mobility in a given gas. The mobilities are constant at low reduced field strengths (E/N) and enable the structure elucidation of biomolecular ions (e.g. peptides). High field mobility measurements can extend our understanding of ion-neutral interactions and of structure changes in molecular ions. Though there are extensive databases on low field mobilities, only little data on high field mobilities exists. In order to study the low and high field mobilities of peptide ions, a home-built IM spectrometer capable of working at reduced pressure (down to 10 mbar), and thus at high E/N (up to 100 Td), was coupled to an infrared matrix assisted laser dispersion/ionization (IR-MALDI) source [1,2].

Experimenteller Teil (max. 120 Wörter)

Two versions of the IR-MALDI source were implemented and compared: In one case, the dispersion and ionization process took place at reduced pressure (RP), inside the IM spectrometer, and in the other case it took place just outside of it, at atmospheric pressure (AP). A heated ion transfer tube for mass spectrometry was used to guide the ions into the low-pressure chamber and as a means for enhanced desolvation. The two source variations were characterized and compared.

Ergebnisse und Diskussion (max. 300 Wörter)

Both source configurations were well-suited for the analysis of peptide ions. The additional transport length for ion desolvation in the AP configuration results in ion losses and slightly lower sensitivity but higher resolution than the RP configuration. Various peptide sequences as well as different isomers (such as linear/cyclized) were measured in both source configurations and their results were compared.

The low field mobilities and collision cross-sections of various peptide ions were determined at intermediate pressure. Structural information was obtained by comparing these values to calculated molecular structures. The latter were determined by molecular dynamics (MD) simulations at high temperature with the aid of the software package GROMACS. A statistical distribution of conformations was then extrapolated for low temperature conditions [3] and an average cross section value in N_2 was determined through the software MOBCAL [4]. The cross-section results from the nanosecond gas phase simulation are in good agreement with the experimental microsecond data. The collision cross-section is an average value stemming from different structures during the ion's flight through the drift tube.

The first high field mobility measurements of peptides are presented as well.

Neue Aspekte (max. 20 Wörter)

First reduced pressure IR-MALDI IM spectrometer, high field mobility of peptides, cross-section determined through statistical distribution of conformations.

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Stichworte (max. 5)

IR-MALDI, ion mobility, structure, peptides, collision cross-sections

Poster for DGMS

Monitoring and correlating of protein charge states with respect to amino acid modification and buffer conditions

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Introduction

Native proteins in solution carry positive and negative charges according to their amino acid sequence. In a typical spherical protein about one-third of the charged amino acids are located on the surface and they interact with the solvent. The charge state of a protein can also be manipulated by biological or chemical modifications [1]. While the charge state of a protein can have a significant influence on its function, it is very challenging to determine it experimentally. To detect the native charge of proteins, measurements need to be conducted under native conditions. The Laser-Induced-Liquid-Bead-Ion-Desorption (LILBID) ionization is a very soft and gentle method which we want to employ for this challenge. The ionization process for the sample is native and there is no active charging of the samples like the standardly used methods e.g. ESI.

Experimental Part

A piezo-driven droplet generator is used to produce droplets of 30 µm diameter with a frequency of 10 Hz. These droplets are transferred into vacuum, where the droplets are irradiated by an IR laser pulse tuned to the absorption wavelength of water (2.94 µm). This leads to the explosive expansion of the droplets, setting the solvated ions free, which can then be mass-analyzed with a quadrupole time-of-flight (Q-TOF) mass spectrometer [2].

The protein is modified chemically with acetic anhydride and propionic anhydride. With the acetylation/propylation of the amino groups in the side chains the charge decreases theoretically with $\Delta Z = -1$ for one modified amino acid [1].

Results and Discussion

We showed that LILBID-MS spectra reflect the native charge states of proteins. The effect of acetylation and buffer conditions is very good to track. We can monitor the differences in charge states under various buffer conditions and modifications. Coupling a LILBID source to a commercial Q-TOF increased our mass resolution 10-fold, as compared to the 1st generation home built instrument. This now allows the differentiation of several acetylation states. We managed to observe the charge state differences between native and modified proteins and are in position to calculate the correlation of charge states between the different variations of the protein. We separated the acetylation states with ion exchange chromatography (IEC) and measured with LILBID. We found the change in average measured charge state ΔZ to be 0.5-0.6. With the IEC we can separate the modification- and charge states of proteins. The LILBID mass spectra are consistent with the IEC results. This work demonstrates that with the LILBID method it is possible to analyze and follow the charge of proteins.

New Aspects

Native analysis of protein surface charge, visibility of charge changing, charge and buffer interactions. Monitoring the charge states of proteins can be used for understanding the functionality of protein complexes.

Keywords:

LILBID QTOF

Native Mass Spectrometry

Protein net charge

Reference

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Elucidation of double bond positions in lipids by means of off-line ozonolysis followed by ultraviolet laser desorption ionization mass spectrometry

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In many physiological processes, the biological activity of lipids is critically determined by the position of the C=C bond in unsaturated carbohydrate chains. One powerful analytical tool to unravel this information is via ozonolysis. This method is used both off-line and on-line [1] and results in the formation of sets of characteristic fragments that unambiguously identify the double bond position. Ozone electrospray ionization (OzESI) and ozone-induced dissociation (OzID) [2] are the most powerful applications of ozonolysis in MS-based lipid analyses. However, the common use of ESI as ionization method limits the technique to more polar compounds. Here we used off-line ozonolysis in combination with silver-assisted UV laser desorption ionization mass spectrometry (UV-LDI-MS) to overcome this limitation.

Experimenteller Teil

A MALDI QStar (AB Sciex) and a MALDI Synapt G2-S (Waters) were used as mass spectrometers. We tested our method for a range of different lipid classes including unsaturated straight chain hydrocarbons (HCs), free fatty acids (FFAs), phospho- and glycosphingolipids, and triacylglycerols (TAGs). As a complex biological sample, a blend of cuticular lipid extracts from *Drosophila melanogaster* was moreover analyzed. To visualize also non-derivatized unpolar compounds (such as alkenes) we used etched silver foils as UV-LDI substrates, giving rise to $[M + Ag]^+$ ions upon LDI with LODs in the low picomole range [3]. Off-line ozonolysis was achieved after transfer of the sample-loaded porous Ag foils into a custom-made chamber for about 30 s (approximate ozone concentration, 2.5 %).

Ergebnisse und Diskussion

For all compound classes, the Ag-UV-LDI-MS method enabled recording molecular $[M+Ag]^+$ ions of the original lipids. Following ozonolysis with 30 s reaction time, the lipids were recorded both as intact molecular species and as the expected characteristic fragments (including in particular aldehydes and carboxylic acids). Even with the relatively low O_3 concentrations as produced by the used simple ozone generator (ACT-300, REDOzone) in the home-built chamber, in most cases a full conversion of the C=C bonds to ozonoides and fragments was obtained within 120 s. The mass spectra of single-component samples of singly or doubly unsaturated standards thus readily resulted in the desired information about the double bond position. In addition to alkenes and unsaturated free fatty acids (e.g., oleic acid), we also achieved good results for triolein, dioleylphosphatidylethanolamine, palmitoyloleoylphophatidylcholine and lactosyl(β) ceramide (d4-18:1/24:1). Due to the increasing number of reaction products, the mass spectra of more complex samples (e.g., cuticular *Drosophila* extract) or of lipids with a high degree of unsaturation were however increasingly difficult to interprete.

In this case, the use of the higher-resolving Synapt mass spectrometer in MS and MS/MS mode provided promising results. Low-energy CID of the formed secondary ozonoides with well-known *m/z* values of the $[M+O_3+Ag]^+$ species led to controlled dissociation of the

compounds at the double bond position and gave rise to essentially the same fragments as obtained via direct ozonolysis but within easy to interprete MS/MS spectra. Taking advantage of this feature, it was for example possible to differentiate 7-C25:1 and 9-C25:1 in a whole cuticular lipid extract from virgin male *Drosophila melanogaster*.

Next to showing the selected application examples we also present results from a time course study which revealed variable reaction rates for different substances. For example, tricosene (9*Z*-C23:1) reacted faster with O_3 than oleic acid (9*Z*-FFA18:1).

Neue Aspekte

UV-LDI-MS method enabling rapid identification of the C=C double bond positions in unsaturated lipids following off-line ozonolysis.

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SIMPLEX reveals myoglobin as a key player in cardiac lipid metabolism

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Cardiovascular diseases are the number one cause of death worldwide. In many forms of heart disease, including diabetic cardiomyopathies, heart failure and ischaemic heart disease, alterations in cardiac mitochondrial energy metabolism contribute to a decrease in cardiac efficiency and to contractile dysfunction. Moreover, elevated deposition of fatty acids into intramyocardial lipids is associated with distinct pathological processes that impair cardiac function. Even though these processes are still elusive, more light sheds on with the recent knowledge on myoglobin's (Mb) function. Previous studies support Mb as a protector of cardiac function in hypoxia and myocardial ischemia/reperfusion-injury [1].

Experimenteller Teil

We applied the previously developed extraction protocol SIMPLEX (**SI**multaneous **M**etabolite, **P**rotein, **L**ipid **EX**traction procedure) [2] on the cardiac muscles from an $Mb^{-/-}$ mouse model as well as the wild-type littermates. In brief the cardiac tissue was incubated with cold MeOH, MTBE was added and water was utilized to induce phase separation. The individual fractions containing lipids (top phase), metabolites (lower phase) and proteins (pellet) were then subjected to the individual omics workflows. Here we demonstrate (i) how SIMPLEX is suited to analyze cardiac tissues, (ii) to investigate the interlinked proteome, lipidome and metabolome at the systems scale, and (iii) to study how myoglobin deletion influences the heart metabolism of mice.

Ergebnisse und Diskussion

The mass spectrometry based lipidome analysis reveals a significant increase in triglycerides with a preferential incorporation of palmitic and oleic acids. The 3-fold higher deposition of lipids in $Mb^{-/-}$ hearts was associated with depressed cardiac function compared to wild-type mouse hearts as assessed by echocardiography. Glycerophospholipid levels as well as the metabolome and proteome related to FA metabolism tend to be unaffected by myoglobin ablation. Our results have important implications to pathophysiological conditions where lipotoxicity is evident and prove the robustness of the SIMPLEX approach to investigate interconnected systems in tissues.

Neue Aspekte

Combinatorial multimolecular omics approach of cardiac tissue.

Referenzen

[1] Rassaf, T. et al. Nitrite reductase function of deoxymyoglobin: oxygen sensor and regulator of cardiac energetics and function. Circ. Res. 100, 1749-1754 (2007).
[2] Coman, C. et al. Simultaneous Metabolite, Protein, Lipid Extraction (SIMPLEX): A

Combinatorial Multimolecular Omics Approach for Systems Biology. Mol Cell Proteomics 15, 1453-1466 (2016).

Title: Lipidomics of Pig Brain Using the PIRL-DIVE Homogenisation Techniqu

Authors: Marceline Manka Fuh, Marcus Wurlitzer, Dominik Schwudke, Nils–Owe Hansen, Dwayne Miller, Hartmut Schlüter

Sample homogenisation in many cases is the first step of the analysis of biomolecules. Many tools have been developed and are commercially available for the homogenisation of biological samples, with each attached to several pros and cons. Desorption by impulsive vibrational excitation (DIVE) is a homogenisation method of the picoseconds infrared laser (PIRL). It is an ultrafast and soft homogenization technique, which has been used for the gentle extraction of proteins from tissues[1]. The goal of this study was to investigate the adequacy of PIRL for the homogenisation of brain tissues for lipidomics.

The brain of a domestic pig was harvested and ablated with the PIRL. The ablation plume was directed into a falcon placed in a nitrogen bath for immediate freezing. Lipid extraction was performed with a protocol adapted from the MTBE extraction method be Matyash *et al*[2]. followed by MS analysis. Direct infusion on the Q exactive was performed whereby both positive and negative nano-electrospray ionisation MS/MS with data dependent acquisition (DDA) was employed for 5 minutes alternately. The resulting data were processed using the LipidXplorer software.

More than 500 lipids were identified from each sample, most of them in the negative ionisation mode compared to the positive mode. The two main abundant lipid classes were glycerophospholipids and sphingolipids. Furthermore PIRL-DIVE extraction of lipids from brain tissue is yielded reasonable reproducible results.

The effficiency of PIRL-DIVE method will be compared to other classical methods of tissue homogenisation in further experiments.

References:

[1]Kwiatkowski, M., Wurlitzer, M., Omidi, M., Ren, L., Kruber, S., Nimer, R., Robertson, W. D., Horst, A., Miller, R. J. D. and Schlüter, H. (2015), Ultrafast Extraction of Proteins from Tissues Using Desorption by Impulsive Vibrational Excitation. Angew. Chem. Int. Ed., 54: 285–288. doi:10.1002/anie.201407669

[2]Matyash V, Liebisch G, Kurzchalia TV, Shevchenko A, Schwudke D. Lipid extraction by methyl-*tert*-butyl ether for high-throughput lipidomics. *Journal of Lipid Research*. 2008;49(5):1137-1146. doi:10.1194/jlr.D700041-JLR200.

Titel

Spotting of Structural Isomer Mixtures of Diacyl-Glycerophospholipids via UPLC-MS/MS

Autoren

Prof. Dr. Wolf-Dieter Lehmann (DKFZ und Biochemie-Zentrum Heidelberg), Katharina Wozny (Biochemie-Zentrum Heidelberg), Prof. Dr. Britta Brügger (Biochemie-Zentrum Heidelberg)

Einleitung

MS/MS spectra are correlated to chemical structure in a fingerprint-like manner. Structural isomers may give rise to MS/MS spectra exhibiting isomer-specific fragment ions or isomer-specific fragment ion abundances. The latter case is realized for mixed diacyl-glycerophospholipids (dGPLs). These carry two different fatty acid residues (A/B) esterified to glycerol positions sn1 and sn2, respectively. Thus, mixed dGPLs occur in the two isomeric structures A(sn1)/B(sn2) and B(sn1)/A(sn2). It is known that upon MS/MS in the negative ion mode these isomers generate MS/MS spectra with fatty acid anion (FAA) fragment abundances that are influenced by the position of the acyl substituents [1]. Here, we use this phenomenon to spot by UPLC-MS/MS isomer mixtures in commercial mixed dGPL standards with defined structure.

Experimenteller Teil

An UPLC-MS/MS Orbitrap system (ACQITY UPLC® coupled to a Q Exactive™ Quadrupole-Orbitrap™, Thermo Scientific) was used. A reversed phase column (CSH™ C18 1.7µm, 1.0x150mm, Waters) was used for separation using a 30 min gradient and MS/MS analyses were performed in negative ion mode. Experiments were set up as cycle between full MS and targeted MS/MS with a sampling frequency of about 4 Hz. This delivered about 100-200 MS/MS scans over a typical phospholipid UPLC peak. Analytes were mixed dGPL standards obtained from Avanti® Polar Lipids. (93 Worte)

Ergebnisse und Diskussion

We investigated a set of mixed dGPLs standards of the classes phosphatidylcholine, phosphatidylethanolamine, phosphatidylglycerol, phosphatidylinositol, phosphatidylserine, and phosphatidic acid by negative ion UPLC-MS/MS. We analyzed pairs of FAA fragment elution profiles according to three criteria, (i) intensity ratio, (ii) intensity difference of normalized profiles, and (iii) retention time. In general, FAA fragment intensities for the abovementioned phospholipid classes are position-specific and thus isomer-specific. A slight UPLC retention time shift in mixed dGPL positional isomers effects that the FAA intensity ratio profile is not constant over the corresponding UPLC peak. We demonstrate demonstrate spotting and composition estimation dGPL isomer mixtures by the ciritera listed above. All three abovementioned parameters qualified for the reliable detection of structural isomers in isomer mixtures. The significance of these parameters was investigated by replicate analyses, by control measurements and by simulations. As a result, cut-off values for each parameter are obtained for differentiation between pure analytes and mixtures of structural isomers. Data evaluation is demonstrated manually as well as by using a dedicated module of the software MassMap®.

Neue Aspekte

Mixtures of structural isomers of synthetic mixed diacyl-glycerophospholipid standards are spotted by regular UPLC-MS/MS

Referenzen

1. Pulfer M, Murphy RC. Mass Spectrom Rev 2003, 22, 332-364. Electrospray Mass Spectrometry of Phospholipids

Stichworte

UPLC-MS/MS, diacyl-glycerophospholipids, negative ion ESI, structural isomer mixtures

Themengebiete

Targeted Lipidomics, Method Development

Profiling von konfigurationsisomeren Phospholipiden mittels HILIC-ESI-MS/MS

Christian Vosse, Heiko Hayen
Westfälische Wilhelms-Universität Münster

Einleitung (max. 120)

Phospholipide (PL) sind aufgrund ihrer unterschiedlichen Funktionen in biologischen Systemen wichtige Lipide. Hauptvertreter sind Phosphatidylcholin, Phosphatidylethanolamin, Phosphatidylserin, Phosphatidylinositol, Diphosphatidylglycerol, Phosphatidylglycerol (PG) und Bis(monoacylglycero)phosphat (BMP). BMP ist ein Konfigurationsisomer des PG, welches vor der Entdeckung 1967 von BODY und GRAY[1] in Schweine- und Rattenlungen fälschlicherweise als PG bestimmt wurde. Das Interesse an BMP wurde aufgrund seiner biochemischen Eigenschaften (ungewöhnliche Selektivität und Bindung der Fettsäuren), seiner Relevanz für zahlreiche biologische Aktivitäten (z.B. Cholesterolhomöostase), seiner spezifischen Zelllokalisation und seiner wichtigen Rolle in verschiedenen Krankheiten (z.B. lysosomale Speicherkrankheit oder Brustkrebs) geweckt.[2][3] Mehrere Studien zeigen die Möglichkeit zur Nutzung des BMPs als Biomarker für verschiedene Krankheiten. Folglich sollen in diesem Beitrag die polaren Lipide aus MCF-7 Brustkrebszellen mittels einer neu entwickelten HILIC-ESI-MS/MS-Methode analysiert werden.

Experimenteller Teil (max. 120)

Die verschiedenen Lipidklassen sowie ihre jeweilige Diversität, welche durch die Bindung von Fettsäuen mit unterschiedlicher Kettenlänge und Doppelbindungsanzahl hervorgeht, erfordern eine leistungsstarke Analysenmethode. Wichtige strukturelle Informationen können mittels der MS und MS/MS erhalten werden. Neben der Molekülmasse können durch Fragmentierung der Ionen die gebundenen Fettsäurereste bestätigt werden. Im Fall der Konfigurationsisomere PG und BMP geben jedoch die MS/MS-Spektren im negativen Ionisationsmodus keine Hinweise zur Unterscheidung beider Lipide. Dies macht eine vorherige chromatographische Trennung notwendig. Für eine Trennung der Lipidklassen anhand der polaren Kopfgruppe wurde eine Hydrophile Interaktionsflüssigchromatographische (HILIC) Methode mit einem binären Gradientensystem entwickelt.

Ergebnisse und Diskussion (max. 300)

Durch den Einsatz der HILIC konnten zehn wichtige Phospholipidklassen getrennt werden. Weiterhin konnte eine Trennung anhand der Kettenlänge der Fettsäurereste erreicht werden. Die Doppelbindungsanzahl hatte keinen Effekt auf die Trennung, wodurch die Differenzierung der Lipidspezies mit benachbarter Doppelbindungsanzahl erschwert wird.

In einigen Krebsarten ist der erbB2 Wachstumfaktorrezeptor überexpremiert, wodurch es zu einer unkontrollierten Zellteilung und so zu Tumoren kommen kann. MCF-7 Brustkrebszellen haben einen genetisch veränderten Wachstumsfaktor (neuT), welcher permanent aktiv ist. Durch die Implementierung eines tet-on-Systems kann die Genexpression durch Zugabe von Doxycyclin aktiviert werden. Zur Demonstration der Anwendbarkeit der Lipidprofiling-Methode wurden mit Doxycyclin behandelte sowie zur Kontrolle unbehandelte MCF-7-Zellen extrahiert, welche vom Leibnitz-Institut für Arbeitsforschung an der TU Dortmund zur Verfügung gestellt wurden. Mit der entwickelten Methode konnte gezeigt werden, dass durch die Doxycyclin-Zugabe eine Verschiebung der gebundenen Fettsäuren der BMP Spezies zu kürzeren Kettenlängen stattfand und sich somit eine deutliche Veränderung im Vergleich zur Kontrollprobe ergeben hat. Dagegen konnte beim PG keine nennenswerte Veränderung festgestellt werden.

Neue Aspekte (max. 20)
Entwicklung einer Lipidprofiling-Methode zur Trennung der konstitutionsisomeren Phospholipide PG und BMP mittels HILIC-ESI-MS/MS.

Referenzen (max. 5)

[1] D. Body, G. Gray, *Lipids* 1 (1967) 253-263.
[2] F. Hullin-Matsuda, C. Luquain-Costaz, J. Bouvier, I. Delton-Vandenbroucke, *Prostag. Leukotr. Ess*. 81 (2009) 313-324.
[3] C. Cadenas *et. al.*, *Biochim. Biophys. Acta* 1821 (2012) 1256-1268.

Stichworte (max. 5)
Brustkrebszellen, HILIC, Phospholipide, Lipidprofiling, BMP

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SelexION® DMS-based detergent interference removal for shotgun-lipidomics analyses

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ABSTRACT

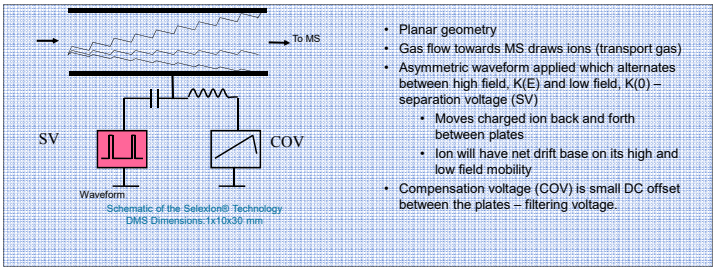
Detergents comprise a critical tool for multiple biochemical and molecular biological applications. For example, they can be used for extracting proteins from tissue samples and stabilizing membrane proteins in solution. They are particularly important for preserving a folded and active state of membrane proteins, which represent the majority of today's drug targets. To fully understand the function of these proteins, in-depth analyses of the bound lipids are required. However, these samples typically contain high concentrations of detergents and are thus often not compatible with mass spectrometric measurements. To date, stringent detergent removal steps are required prior to MS analyses that may alter the amount or ratio of the present lipid classes and species.

SelexION® technology can separate isomeric and isobaric analytes based on their dipolar moment as well as filtering chemical noise from a sample. Here we apply the SelexION technology to remove chemical interferences, namely a range of different commonly used detergents molecules from a lipid sample. This allows measurements of a detergent-contaminated lipid sample by the direct infusion shotgun method without involved sample workup, thus protecting the MS instrumentation from contamination and allowing the infusion of larger amounts of sample extracts without sacrificing dynamic range to the unwanted high-abundance detergents signals.

ABSTRACT

Detergents comprise a critical tool for multiple biochemical and molecular biological applications. For example, they can be used for extracting proteins from tissue samples and stabilizing membrane proteins in solution. They are particularly important for preserving a folded and active state of membrane proteins, which represent the majority of today's drug targets. To fully understand the function of these proteins, in-depth analyses of the bound lipids are required. However, these samples typically contain high concentrations of detergents and are thus often not compatible with mass spectrometric measurements. To date, stringent detergent removal steps are required prior to MS analyses that may alter the amount or ratio of the present lipid classes and species.

SelexION® technology can separate isomeric and isobaric analytes based on their dipolar moment as well as filtering chemical noise from a sample. Here we apply the SelexION technology to remove chemical interferences, namely a range of different commonly used detergents molecules from a lipid sample. This allows measurements of a detergent-contaminated lipid sample by the direct infusion shotgun method without involved sample workup, thus protecting the MS instrumentation from contamination and allowing the infusion of larger amounts of sample extracts without sacrificing dynamic range to the unwanted high-abundance detergents signals.



MATERIALS AND METHODS

Lipid standards and detergents were purchased from Anatrace, Sigma and Avanti Polar Lipids. Lipid standards, detergents and dried extracts were reconstituted in CH_2Cl_2/MeOH 1:1 with 10mM Ammonium acetate and introduced by direct infusion using a syringe pump into a SCIEX TripleTOF® 6600 mass spectrometer system equipped with a SelexION technology device.

The samples were measured by MS-TOF acquisition mode. SelexION technology parameters were 4100V Separation voltage, Resolution gas 10-25, and Isopropanol as modifier with modifier composition set to "low". Compensation Voltage (CoV) was ramped over a range from -30 V to +40 V.

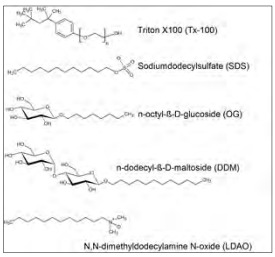


Figure 1 Structures and names of the detergents analysed in this study. Triton X100 contains a Polyethylenglycol-side chain of varying chain length. SDS is a widely used detergent used for protein extraction procedures. Octyl glucoside and mannose glucoside are non-ionic surfactants used for solubilizing integral membran proteins and dimethyl dodecylamine oxide is a micelle-forming surfactant also used for stabilization of membrane proteins.

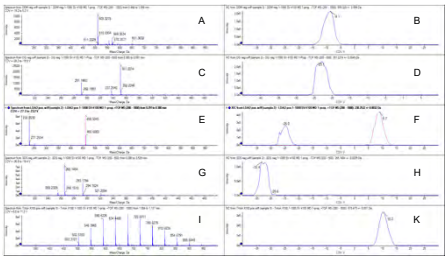


Figure 2: Full-MS spectra (A,C,E,G,I) and Ionograms (B,D,F,H,K) of the detergents. A,B: DMM, C,D: OG; E,F: LDAO; G,H: SDS; I,K: Triton X100. Separation voltage was set to 4100 V and samples where introduced with n-propanol in the carrier gas at 280 ul/min.

Neutral detergent molecules ionize as [M-H]- and [M+OAc]- in negative mode (DMM and OG). LDAO forms a dimer and can be seen as [M+H]+ and [2M+H]+. SDS ionizes as [M-H]-. Triton X-100 is a mixture of different degees of polymerization.

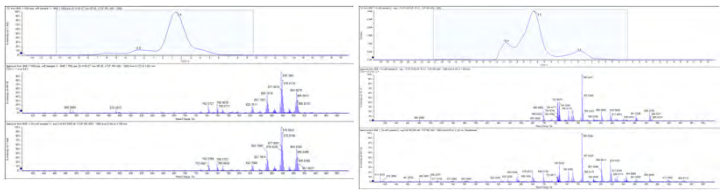


Figure 3: Full Scan MS spectra of the bovine heart lipid extract in positive mode (A-C) and in negative mode (D-F). A and D show the ionogram with the compensation voltages (CoV) rampled. B and E show the summed MS spectrum over the CoV range highlighted in blue. As comparison, C and F show the Full MS spectra of the same extracts with the SelexIon cell turned off.

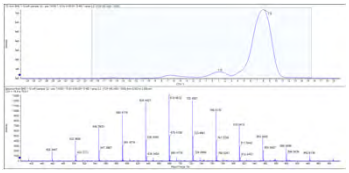


Figure 5: Lipid extract contaminated with **Triton X100** in positive mode. The upper panel shows the ionogram, the lower panel shows the composite spectrum across the blue CoV region of the upper panel

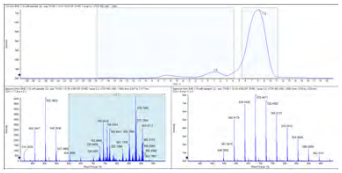


Figure 6: Lipid extract contaminated with **Triton X100** in positive mode. The lower panel shows the composite MS CoV-peak at 7.8V contains exclusively signals of Triton X-100, whereas the hightlighted region between -18V – 4V contains the lipid signals. Some minor overlap between lipids and Triton signals is evident (circled peaks).

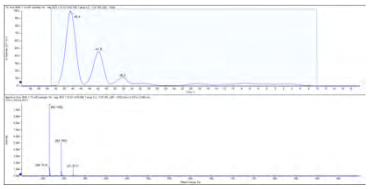


Figure 7: Lipid extract contaminated with **SDS** in negative mode. The three prominent CoV-peaks at -48V, -42V and -36V correspond to the three different SDS masses seen in the spectrum in the lower panel. The strong SDS signal is occupying most of the dynamic range of the detector.

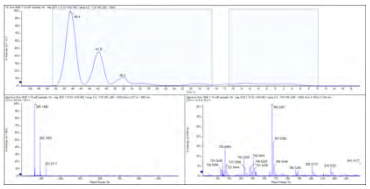


Figure 8: Removing **SDS** contamination from the ion beam using SelexIon-Technology. The composite MS spectrum in the lower left panel shows that the CoV-region between -53V to -15V exclusively contains SDS signals, whereas the hightlighted region between -11V to 10V contains the lipid signals.

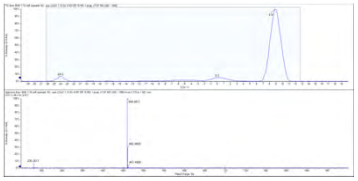


Figure 9: Lipid extract contaminated with **LDAO** in positive mode. The two prominent CoV-peaks at -24V, and -8.9V correspond to the [M+H]+ and the [2M+H]+ species respectively. The lipid signals are obliterated by the detergent signals which occupy a large part of the dynamic range.

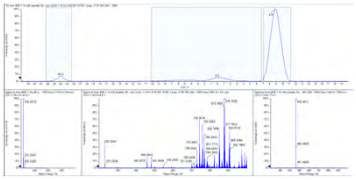
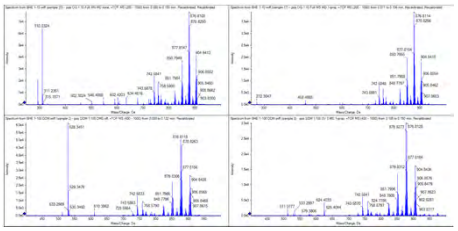


Figure 10: Removing **LDAO** contamination from the ion beam using SelexIon-Technology. The composite MS spectrum in the lower leftand right figure shows that the CoV-region containign tyhe LDAO signals, whereas the middle region between -11V to 10V contains the lipid signals.

Figure 11: Removal of detergent interference using the proton affinity effect. Proton affinity is often exhibited by the modifier solutions, in this case 1-propanol, and is a measure of gas-phase basicity. Surprisingly, it can be used to the advantage of removing the positive charge from the detergents. In this experiment, no separation or compensation voltage was applied, but the modifier was added to the carrier gas as in the previous experiments.



In the upper two figures, the lipid extract was contaminated with OG (circled peak) and in the lower figures the lipid extract was contaminated with DMM (circled peak). In the left figures the DMS was turned off and in the right figures, 1-propanol was infused into the DMS cell. The signals of the detergent molecules are completely eliminated, avoiding a contamination of the mass spectrometer.

CONCLUSIONS AND SUMMARY

Detergents pose a challenge in many analytical workflows in mass spectrometry, but are often critically required for biochemical sample preparation. For example, membrane proteins typically require detergents for retaining stability and their physiological function. We have added the most commoly used detergents at a concentration above their respective CMC to a commercially available bovine heart lipid extract. These detergents included both ionic detergents (SDS, LDAO) and non-ionic detergents (OG, DDM and Triton X-100).

The mass spectra showed partial to total masking of the lipid signals in direct infusion measurements, as outlined in Figures 3-10. Using the SelexION® technology, we show that specific compensation voltages can be used to separate or dramatically reduce the detergent interference for the lipid signals, making a direct shotgun based analysis of these solutions possible.

This has a twofold benefit. Firstly, it prevents the mass spectrometer hardware from contamination. Often, detergents concentrations can be very high and this inevitably leads to a contamination of the front quadrupoles in the mass spectrometers, which requires a lengthy and disruptive cleaning of the instrument front end. In the case of the lipid extract shown here, CoV values for the detergents were sufficiently separated from the lipid CoV values, allowing an almost quantitative elimination of the detergent signals.

Secondly, the interfering signals from the detergents can be very large compared to the signals of the analytes of interest. This would limit the available signal/noise for the analytes of interest. By removing the strong interfering signal, more dynamic range is available for the interesting analytes, making the method more sensitive.

In summary, we show that SelexION Technology significantly improves the analysis of a lipid extract by shotgun lipidomics. It should be noted that this workflow is also applicable to other analyte classes which are routinely contaminated with detergents. This method may be particularly useful for the direct lipidomic analysis of membrane protein extracts with high detergent concentrations, and thus allow direct analyses of lipids required for stability and physiological function of these proteins.

TRADEMARKS/LICENSING

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Bestimmung von Doppelbindungspositionen in Lipiden mittels photochemischer Nachsäulenderivatisierung und Tandem-MS

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Einleitung

Lipide umfassen eine Gruppe von Biomolekülen, die eine große Variation an chemischen Strukturen aufweisen und verschiedenste Aufgaben und Funktionen in unterschiedlichsten Lebensformen besitzen. Doppelbindungen haben Einfluss auf die chemischen, biochemischen und biophysikalischen Eigenschaften der Lipide. Die Lokalisation von Doppelbindungspositionen ist eine Herausforderung hinsichtlich der Komplexität der Strukturen bzw. der vorliegenden Gemische. Die photochemische Paternò-Büchi-Reaktion wurde unter Bildung von Acetonaddukten und daraus resultierender diagnostischer massenspektrometrischer Fragmentionen zur Bestimmung von Doppelbindungspositionen eingesetzt.[1] In diesem Beitrag wird diese Methode mit der HPLC-Trennung erweitert und die Anwendbarkeit auf Lipidgemische und komplexere Lipide demonstriert.

Experimenteller Teil

Die Paternò-Büchi-Reaktion erfolgte im Rahmen einer Nachsäulenderivatisierung über eine Exposition mit UV-Licht in einem photochemischen Reaktor unter Bereitstellung eines konstanten Acetonstroms zusätzlich zu der mobilen Phase. Zur Optimierung der Online-Reaktion wurden Parameter wie die Reaktionszeit und die konstante Flussrate des Derivatisierungsreagenzes Aceton variiert. Als Modellsubstanz wurde die einfach ungesättigte Ölsäure eingesetzt. Im Weiteren wurde die Anwendbarkeit der Methode auf Monoolein und einem Lipidgemisch aus einem Bis(monoacylglycero)phosphat und Phosphatidylglycerol (PG) unter Betrachtung einer Kopplung der Methode mit einer HPLC-Trennung demonstriert.

Ergebnisse und Diskussion

Mit Exposition mit UV-Licht (254 nm) konnte, neben dem deprotonierten Molekül der Ölsäure, das entsprechende Acetonaddukt mit einer Massendifferenz von 58 Da detektiert werden, welches der Reaktion von Aceton mit der Doppelbindung der Fettsäure unter Ausbildung eines

Oxetans zugrunde liegt. Über MS/MS-Experimente wurden diagnostische Fragmentionen gebildet, welche eine eindeutige Lokalisation der Doppelbindung ermöglichten.

Ausgehend von den optimierten Bedingungen für die Reaktion wurden Experimente mit komplexeren Lipiden und Lipidgemischen durchgeführt. Beginnend mit Monoolein, dem Glycerinester der Ölsäure, konnten analoge Ergebnisse zu denen der Ölsäure erzielt werden. Die Fragmentierung resultierte zunächst in der Bildung der freien derivatisierten Ölsäure, welche nach weiterer Fragmentierung zu den diagnostischen Fragmenten führte. Eine erfolgreiche Kopplung der HPLC mit der Online-Reaktion wurde anhand eines Lipidgemisches aus Standards von BMP- und PG demonstriert. BMP und PG stellen Konstitutionsisomere dar, dessen Differenzierung eine HPLC Trennung erfordert. Nach erfolgreicher Trennung der beiden Isomere erfolgte die UV-Reaktion mit Aceton unter Ausbildung der Acetonaddukte. Die Fragmentierungsexperimente erfolgten analog zu denen der Paternò-Büchi-Produkte der Monooleinsäure und ermöglichten die Bestimmung der Doppelbindungsposition.

Neue Aspekte

Lokalisation von Doppelbindungen in Lipiden über eine photochemische Online-Reaktion, der Paternò-Büchi-Reaktion, und Tandem-MS, sowie Kombination der Methode mit einer HPLC-Trennung.

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Stichworte (5)

Lipidanalytik, Doppelbindungsposition, Paternò-Büchi-Reaktion

In situ monitoring of lipid oxidation using electrochemistry-mass spectrometry coupling

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Introduction

Lipid peroxidation products (LPPs) generated by oxidative stress have been recognized as biomarkers of numerous human disorders including atherosclerosis, neurodegenerative diseases, type 2 diabetes, chronic inflammation and aging. LPPs are highly diverse in their structure, stability, reactivity and, as a result, in their biological functions. Such chemical diversity makes it challenging to study LPPs in biological samples and especially to identify reactive early oxidation products giving rise to the large variety of LPPs. However, characterization of the initial oxidation steps is important to understand the pathology onset and might assist the development of possible therapeutic interventions.

Experimental section

Here we applied electrochemical (EC) oxidation, a micropreparative technique allowing fast simulation of biological and technological redox reactions, coupled on-line to mass spectrometry (MS) for detection of *in situ* generated early oxidation products from two different phospholipids. 1-palmitoyl-2-linoleoyl-*sn*-glycerophosphatidylethanolamine (PLPE) and N-(octadecenoyl)-sphing-4-enine-1-phosphocholine (SM) were oxidized using ROXY EC system (Antec, Leyden, NL) equipped with a boron doped diamond (BDD) working electrode and coupled on-line to ESI-ion trap MS.

Results and discussion

The voltage-dependent oxidation of PLPE and SM lipids infused into the µ-PrepCell was first monitored by ramping the voltage (0 to 3.2 V) or just switching the EC-cell on and off (0 and 3 V). We were able to detect profound changes in the electrospray mass spectra (ESI-MS), more specifically the decline in the signal of protonated ions, $[M+H]^+$ of the non-modified phospholipids, and concomitant appearance of new signals attributed to EC generated products. Thus, nine oxidation products formed due to oxygen addition (or products due to the addition of 9 oxygen atoms?) and seven products formed due to oxidative cleavage were detected for PLPE. Interestingly, *in situ* monitoring of PLPE oxidation allowed to detect not only relatively stable hydroxyl- and carbonyl-derivatives but also short lived unstable hydroperoxides. EC oxidation of SM lipid resulted in five oxidation products formed due to oxygen addition, including

hydroperoxy, hydroxy and carbonyl species as well. Furthermore, using on-line oxidation monitoring we demonstrated that four main SM oxidative cleavage products were formed by the oxidative degradation of sphingosine moiety. Additionally, by introducing the reaction coil between EC cell and ESI source, reactivity of electrophilic early oxidative products towards nucleophilic substrates (glutathione) was evaluated.

Novel aspects

On-line coupling of electrochemical oxidation to MS allows *in situ* monitoring of lipid peroxidation.

Keywords

electrochemical oxidation, mass spectrometry detection, lipid oxidation

Enabling High-Confidence Human Endogenous Metabolite Identification via High-Resolution MS/MS Retention-Time Library

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Metabolite identification remains a major bottleneck in metabolomics. Our work focuses on building a human metabolite library. It contains multiple layers of information including accurate masses, high-resolution MS/MS spectra and normalized retention time in both RPLC and HILIC separations. We also illustrate the application of this library for rapid metabolite identification in human biofluids.

Experimenteller Teil

831 standards were obtained from the Human Metabolite Database (HMDB). These were analyzed via a Dionex RSLC (Thermo Fisher) and detected by an impact HD Q-TOF MS (Bruker Daltonics). For retention time measurement, metabolite standards were pooled into mixtures. Each mix was spiked with a retention-time standard and separated on a RP or HILIC column.

Ergebnisse und Diskussion

MS/MS spectra acquired in positive and negative ion modes were manually curated before adding to the library. The addition of retention-time information significantly improved the identification confidence, especially for low intensity or isobaric compounds and isomers. 20-minute linear solvent gradients for reversed-phase (RP) and hydrophilic interaction (HILIC) separation were established. We pooled 32 compounds which were evenly spaced during the separations as a retention-time (RT) standard mixture. Reproducibility of the gradient was assessed using this mixture, and the RT standard deviations were found to be within ±1.3 seconds (n = 5).

Untargeted LC-MS/MS analyses were performed on urine and serum to illustrate the performance of this library. Matching both MS/MS spectra and retention time enabled rapid and high-confidence identification of compounds in both matrices.

Neue Aspekte

High-confidence identification of human endogenous metabolites using high-resolution MS/MS retention-time library

Boosting compound identification confidence in Metabolomics by exploiting all available Q-TOF high resolution accurate mass spectral information.

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Confident compound identification is still one of the major bottlenecks in metabolomics. Ongoing efforts to refine the definitions and levels of metabolite identifications that were first proposed by the MSI initiative stress that higher levels of identification confidence can be reached by joining accurate measurement technology, orthogonal molecular features, and sophisticated software tools.

Experimenteller Teil

Methanolic extracts of three mutant and one wildtype C. glutamicum strain were diluted and separated using an UltiMate RSLC (Thermo Scientific). The LC was coupled to an impact II QToF-MS (Bruker). HRAM MS & MS/MS spectra were acquired by data dependent MS/MS. MetaboScape was used for automatic identification of known target compounds, identification of unknowns, statistics, and pathway mapping.

Ergebnisse und Diskussion

We could highly improve the quality of compound identifications in a study investigating the arginine biosynthesis in C. glutamicum conducted by LC-QTOF non-targeted metabolomics. The developed tools were used to create annotations throughout increasing confidence levels: First, for all compound spectra molecular formulas were generated based on accurate masses, true isotopic patterns, and in-source fragmentation patterns, applying metabolomics-tailored rules and filters. Afterwards, public chemical databases were queried to find structural candidates for the generated molecular formulas of interesting features. Then, a customized analyte target list was applied to additionally exploit retention times of expected features. Lastly, MS/MS spectral library comparisons and in-silico fragmentations enabled to create and verify identifications based on MS/MS fragmentation patterns.

Neue Aspekte

Strategy to achieve highest confidence in compound identifications based on LC-HRAM-MS/MS spectral information using an integrated “turnkey” solution.

Identification and quantification of N-acyl homoserine lactones involved in bacterial communication by matrix-assisted laser desorption/ionization mass spectrometry

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N-Acyl homoserine lactones (AHLs) are bacterial signal molecules of high relevance for both biological and medical research. Being part of the quorum sensing communication system of gram-negative bacteria, AHL play a major role in the regulation of biofilm formation and virulence [1]. Despite various efforts that have been made to analytically determine AHL quantities, previously reported mass spectrometry-based approaches lack applicability for high-throughput assays of biological samples [2]. We investigated matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS) as a tool for quantitative AHL analysis. To facilitate the analysis of low-molecular mass AHLs, novel ionic liquid matrices (ILMs) were assessed in a comprehensive screening [3,4]. Acquisition of quantitative data was achieved by employing isotope-labeled internal standards synthesized in microscale procedures.

Experimenteller Teil

The study included the synthesis of various AHL standard molecules. Synthesis was carried out employing solid-phase as well as solution-phase chemistry in microscale synthesis approaches. Obtained AHL standards were analyzed by MALDI-TOF MS and structurally elucidated by tandem mass spectrometry (MS/MS) methods. ILMs were prepared with equimolar amounts of an acidic MALDI matrix and a counter base. From a screening of approximately 100 ILM preparations, most promising candidates in respect of analyte signal intensities were selected for further evaluation. The performance of synthesized ^{13}C-labeled AHLs in quantitative experiments was assessed by MALDI MS. For this purpose, dilution series of commercial AHL standards were spiked with internal standards and the accuracy of acquired standard curves was evaluated.

Ergebnisse und Diskussion

For a precise determination of quantities of low-molecular mass compounds from biological samples by mass spectrometry, individual isotope-labeled internal standards of all analytes of interest are of great benefit. To enable fast and reliable generation of isotope-labeled AHL standards, a rational synthesis design was employed to transfer complex organic chemistry reactions into microscale procedures. This approach is considerably cost-efficient and can easily be implemented in every analytical laboratory. The microscale synthesis protocols developed in this study were successfully used to produce ^{13}C-labeled standards of all three structural AHL types with yields sufficient for quantitative MS approaches (synthesis yields approx. 10%). Microscale derived AHL synthesis products were only concentrated by solid-phase extraction and required no extensive purification. Application of the isotope-labeled standards in quantitative MALDI MS experiments allowed an accurate quantification of AHLs. The obtained data revealed a broad overall dynamic range, reaching lower pico-molar amounts as the limit of quantification. Also, the developed MALDI MS methods proved advantageous for the fast screening and quantification of numerous samples. To further the analytical capabilities of the MALDI MS-based approach, two ionic liquid matrices were introduced, both based on the matrix a-cyano-4-hydroxycinnamic acid (CHCA) and the

counter base 2-aminopentane (AP). The prepared ILMs, *mono*-AP-CHCA and *di*-AP-CHCA, facilitated the MALDI analysis of low-molecular mass AHLs by suppression of interfering matrix background signals. Furthermore, measurements of AHL reference dilution series in *mono*-AP-CHCA without an internal standard revealed a robust linearity between analyte ion intensities and AHL amounts on-target, showing the potential of the ILM as an alternative MALDI matrix for quantification of AHLs. The results of this study indicate a high usability of the developed preparative and analytical techniques to determine AHL concentrations in biological samples, and may allow to gain further insights into AHL-based quorum sensing.

Neue Aspekte

A fast and convenient methodology for the quantitative MALDI MS analysis of bacterial AHL signaling molecules.

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Application of laser ablation for tissue metabolomics

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Metabolomics is one of the big Omics Sciences for the analysis of metabolites. This important class of molecules can be used for biomarker screening in various diseases. Low concentrations and rapid conversion of metabolites e.g. due to oxidation cause problems for their accurate quantification, therefore sample preparation is key in studying these molecules. To optimize metabolite extraction we compare three methods: classic homogenization followed by methanol extraction and two laser extractions, PIRL (Picosecond Infrared Laser) and Er: YAG laser. Here the biomolecules are rapidly transferred from the tissues into a gas phase and the resulting plume is captured on a borosilicate filter.

Experimenteller Teil

5 Organs (liver, pancreas, muscle, brain and kidney) were collected from 3 male C57BL/6J mice. The obtained organs were divided into 3 comparable pieces and the analytes were extracted as described above. All obtained extracts are analyzed by LC-MS/MS and FIA-MS/MS using the Biocrates p180 kit, allowing the quantification of 184 metabolites. Quality control and statistical analysis on the obtained data was performed with MetIDQ (Biocrates) and Perseus.

Ergebnisse und Diskussion

The detected metabolites belong to five different classes: acylcarnitines, amino acids, biogenic amines, hexoses and phospho- and sphingolipids of which 53 were absolutely and 151 relatively quantified. Laser ablation of tissues allowed the extraction, analysis and quantification of 184 metabolites, using the p180 kit. The capture of the ablation plume on a borosilicate filter is compatible with direct analysis by the kit, extraction steps are not necessary. This extraction method also allows the use of less starting material and the storage of the sample on the filter is convenient. The yield difference between the two lasers can be explained by the heat transfer caused by the Er:YAG laser that can damage the molecules, whereas the short pulse duration from PIRL prevents heat transfer and therefore, damage from happening.

Neue Aspekte

Metabolite extraction by PIRL for less molecule damage.

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Quantitative turnover analysis of chlorophylls, carotenoids and tocopherol in green leaves by LC-MS and FTICR-MS

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Abstract: Chlorophylls and carotenoids are belonging to the photosynthetic pigments in chloroplasts of plants playing central roles in light absorption and photoprotection. Synthesis and degradation of photosynthetic pigments (chlorophylls and carotenoids) have been mostly studied in leaves during greening or senescence but not in mature leaves. The question how much biosynthesis and degradation of different photopigments occurs in photosynthesizing green leaves is still open. In order to gain insight into photopigment turnover of mature leaves we conducted long-term $^{13}CO_2$ labelling with peppermint (*Mentha x piperita*) and analyzed the $^{13}C/^{12}C$ signature of chlorophylls (Chls), carotenoids and tocopherols (Toc) by LC-MS and FTICR-MS.

Materials and Methods: Peppermint plants were cultivated in a $^{13}CO_2$ containing atmosphere for 34 d [1]. Hereupon they were transferred to ambient CO_2 where samples were collected from mature leaves over 7 days. Leave samples from day 0, 1, 2 and 7 were extracted and analyzed by LC-PDA-ESI(+)-MS using a C30 column. High resolved FTICR mass spectra were obtained from some exemplary samples in order to distinguish peaks of pigment isotopomers from those of co-eluting matrix compounds and to assign mass peaks to distinct empirical formulae. The ^{13}C degrees of labelling (DoL) of various photopigments over time were determined from the mass spectra. Additional MS/MS experiments were performed to gain insight into the position of ^{13}C in the photopigment molecules.

Results: The main photopigments in peppermint extracts were Chls a and b, α-Toc and the xanthophylls lutein, zeaxanthin, antheraxanthin, neoxanthin (Neo) and violaxanthin and finally β-carotene (β-Car). While Chls and α-Toc predominantly formed $[M + H]^+$ adducts in the positive ESI mode, $[M]^+$ and $[M + H - H_2O]^+$ adducts were additionally detected for carotenoids. After clearing up the mass spectra from matrix compound derived peaks DoLs were determined. Their time courses showed a high turnover for Chl a and β-Car, a lower non-linear decline in DoL for xanthophylls but almost no change in the DoL for Neo. A distinct maximum peak in the mass spectra of α-Toc from day 1 – 7 located between the extreme values for non-labelling and full labelling indicated a recycling of the phytol moiety during turnover of α-Toc [2]. MS/MS experiments supported this hypothesis. Further results concerning turnover of Chls and xanthophylls will be also presented and discussed in the biological context.

New Aspects: Regulation of photopigment metabolism in mature leaves

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Keywords: Turnover of photopigments, ^{13}C labelling, LC-MS, FTICR-MS

Application of LC-MS technique for intra-thallus profiling of polyphenolics in three species of fucoid algae

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Keywords: phlorotannins, brown algae, LC-MS

Introduction

Brown algae possess a unique group of polyphenolic secondary metabolites – phlorotannins, which apparently contribute to multiple physiological functions like herbivore deterrence, UV protection, cell wall formation and bioadhesion. These compounds are acetate-malonate derived polymers of phloroglucinol with different degree of polymerization leading to a wide range of molecular sizes (126 Da to 650 kDa). Depending on the nature of the linkages binding the polymers and on the number of hydroxyls, six major classes of phlorotannins have been defined [1]. A diversity of phlorotannin molecules and their ability to form multiple isomeric structures hamper their detailed analysis. Here we study phlorotannin profiles in different thallus zones of algae to elucidate the connection between allocation and physiological functions of different phlorotannin species.

Experimental section

Three representatives of the order Fucales (*Fucus vesiculosus*, *F. serratus* and *Pelvetia canaliculata*) were used as objects. Samples were taken from four thallus zones of each alga – thallus base, middle zone, vegetative apices and mature receptacles. Plant material was ground and extracted five times with 70% acetone. The acetone was evaporated and remaining water extract was purified via liquid-liquid separation with dichloromethane and then with ethyl acetate [2]. Chromatography was performed on Agilent 1100 instrument equipped with a C18 column (Gemini). MS data were acquired on Bruker Esquire 3000 Plus ESI ion trap mass spectrometer.

Results and discussion

The total amount of soluble phlorotannins varied from 5 to 24% DW and did not differ significantly between three algal species. Receptacles contained approx. 2-fold lower level of polyphenolics than vegetative tissues. Maximum phlorotannin content was found in the middle zone of the thallus for *F. vesiculosus* and in the vegetative tips - for the other two species. All the samples contained phlorotannins with the degree of polymerization (DP) varying from 3 to 50, presumably belonging to the classes of fucols and fucophlorethols. Mass spectrometry data allowed identification of more than 70 phlorotannins. The low molecular weight phenolics dominated in *F. vesiculosus*, and *P. canaliculata* had the maximum relative content of larger molecules (DP>20), which is consistent with literature data [4]. In all three algal species the small-sized phlorotannins (DP 3-8) were concentrated in the vegetative apices, where they presumably act as antioxidants and UV-protectors. The higher molecular weight polyphenols were more specific for middle and basal thallus zones where they might contribute to antifouling

activity and cell wall rigidification. Such a profile of phlorotannin distribution was especially prominent for the subtidal species *F. serratus*.

The research was supported by the Russian Foundation for Basic Research (project no. 17-04-01331)

Novel aspects

Fucus serratus and two more fucoid species accumulate low molecular weight phlorotannins in the vegetative apices.

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UPLC-ESI-QTOF-MS based chemical profiling of *Actaea racemosa* L. (black cohosh) rhizomes to investigate differences in cultivation, wild harvest, and genotypes

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Abstract:

The popular North American medicinal plant *Actaea racemosa* L. (black cohosh) is one of the most widely used herbal remedies. Wild-harvest of the perennial (rhizomes) in multi-tons has led to endangerment of the natural population [1,2]. Therefore government organizations and manufacturers make efforts to cultivate *A. racemosa* in a commercial scale [3,4]. Nevertheless, different genotypes of *A. racemosa* exist [5], and the environment of cultivation may have an influence on the plant's metabolic composition. This, in the end, may result in varying and not reproducible pharmacological activities of herbal products.

The aim of this study is to chemically profile specimens of *Actaea racemosa* rhizome from cultivation, wild-harvests, and from different geographical origins. From LCMS experiments followed by computational investigation of the data we infer chemical differences between the samples. Furthermore, we want to explore genotypes of *A. racemosa* and assign our samples to metabolomic groups.

We analyzed methanolic extracts of a set of 45 rhizome samples of *Actaea racemosa* rhizome, in which you find commercial composite batches from wild-harvests, individual samples from wild-harvests in the US, and samples from different world wide sources, cultivated in same environment in Berlin. Metabolomic data was generated by UPLC-ESI-QTOF-MS analyses. For data analysis open-source, as well as proprietary MS data analysis software was applied. Multivariate statistical analyses were carried out to investigate possible differences between samples of *A. racemosa* rhizome.

Within the investigated sample set, generally, plants from wild-harvests showed overall higher contents in secondary metabolites. The chemical composition of cultivated plants showed clear differences in comparison to the wild-harvested. Within the set of cultivated

plants, samples clustered in distinct groups, supporting the assumption of the existence of different genotypes in the *Actaea racemosa* L. species.

Acknowledgements:

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Metabolomics to study the “war” between plants and insects - Systemic defense induction and post-ingestive rearrangement of plant toxins in insects.

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17-hydroxygeranyllinallool diterpene glycosides (HGL-DTGs) are secondary metabolites in N. attenuata defending tissue against the herbivore M. sexta. Gene manipulation followed by software based metabolite identification enabled characterization of glycosylation in the HGL-DTG pathway in tobacco and clarified the impact on chemical rearrangements with other pathways when ingested by M. sexta.

Experimenteller Teil

Leaf tissue from genetically silenced lines of N. attenuata and frass of 2nd instar M. sexta larvae were extracted with 80% methanol. Extracts were separated with an RSLC (Thermo Fisher). MS analysis was performed by Q-TOF MS (impact II, Bruker). MetaboScape was applied for identification of novel secondary metabolites, automatic identification of target compounds, statistics, and pathway mapping

Ergebnisse und Diskussion

We characterized silenced rhamnosyl and glucosyltransferase lines IRrt1, IRgt1 and IRgt2 impaired in the glycosylation of HGL-DTGs. Metabolite profiling rapidly determined a complete loss of rhamnosylated HGL-DTGs in IRrt1 and the appearance of 12 novel intermediate products in IRgt1 and IRgt2. Feeding assays and screening excreta of M. sexta elucidated the defensive capabilities of HGL-DTGs. 55 novel HGL-DTG-like compounds with different decorations (like caffeoyl moieties) and further deglycosylation products were found. HGL-DTGs with caffeoyl moieties could only be detected in frass of caterpillars directly feeding on N. attenuata plants and not in frass of caterpillars feeding on detached leaves. This indicates that other systemically-induced defensive pathways play a crucial role in the process of detoxification or that HGL-DTGs are used to detoxify potential poisonous metabolites.

Neue Aspekte

MS based metabolite profiling strategies elucidate post-ingestive rearrangement detoxification mechanisms of plant secondary metabolites in insects.

A step forward in GC-HRAM-MS based metabolomics - A novel atmospheric pressure GC-APCI Source increases quantitative and qualitative performance

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Common requests in GC-MS based metabolomics are an increased sensitivity for detecting metabolites and for identification of unknown compounds. Electron ionization (EI) is the standard ionization for GC-MS. Soft ionization by atmospheric pressure chemical ionization preserves molecular ion information enabling identification of unknowns, a reason why GC-APCI became more popular recently.

Experimenteller Teil

Standards and cell culture supernatants of MiaPaCa-2 pancreatic cancer cells were derivatized and samples were separated using a Rxi-5ms (Restek) GC column which was coupled to a novel APCI source and analysed in an oTOF-MS (micrOTOF , Bruker Daltonics). Data was acquired with a rate of at least 3 spectra per second. PFTBA was injected into the APCI source as a calibrant for data recalibration.

Ergebnisse und Diskussion

Here we will report the application of a novel GC-APCI source design coupled with a high resolution, accurate mass oTOF to analyse derivatized metabolite extracts and reference standards. In comparison with earlier results, the analytical performance could be improved resulting in a higher number of compounds identified in human cancer cell extracts. Additionally, lower limits of quantification in the sub-micromolar range were found for twenty metabolites. At the same time, the analytical linear response range was either maintained or slightly increased.

In summary, the novel GC-APCI source is expected to reveal more significantly regulated metabolites in metabolomics research and to enable their sensitive quantification by low LLOQs, broad linear ranges and decreased relative standard deviations of replicates analyses.

Neue Aspekte

Improved sensitivity and unknown ID capabilities in GC-MS based metabolomics by novel GC atmospheric pressure chemical ionization (APCI) source.

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ptble
Universität Hamburg
DER FORSCHUNG | DER LEHRE | DER BILDUNG
GALAB

Discrimination of apple and potato cultivars by non-targeted metabolomic fingerprinting via UPLC-IMS-QToF analysis

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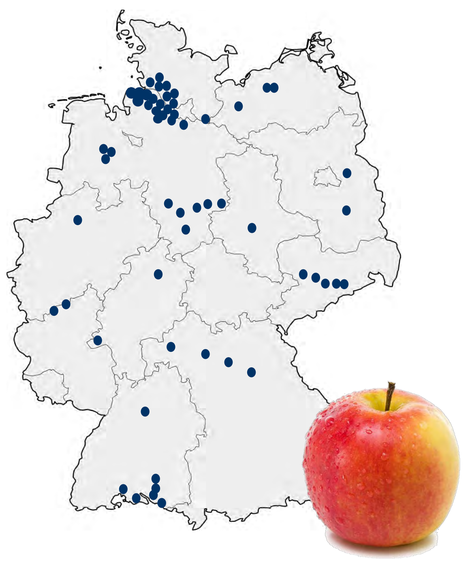
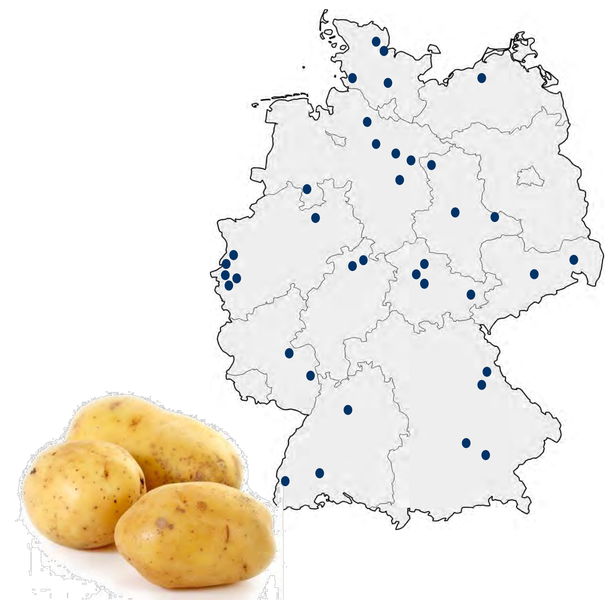
Introduction

In recent years an increasing demand for regional products could be noticed. Consumers are prepared to pay higher prices for commodities with a certain geographical origin. As a consequence the market price fluctuates depending on the origin of the goods. Unfortunately it is not uncommon that apples and potatoes are imported and sold with incorrect information. To detect the fraud analytical methods for food authentication became an important issue. Non-targeted metabolomics approach focus on the analysis of as many metabolites as possible (fingerprint) to differentiate between commodities with different origin or of different cultivar by comparing metabolite patterns.



Materials and Methods

Authentic potatoes and apples of known geographical origin were collected in 2016 from the most important German growing areas. About 200 samples per food matrix including 5 to 15 cultivars were cryomilled with dry ice and subsequently lyophilized. After extracting the homogenates with polar and nonpolar solvents the samples are transferred to the UPLC-QToF. The obtained data sets are aligned and evaluated via multivariate data analysis. e.g. Principal Component Analysis (PCA).



Conclusion

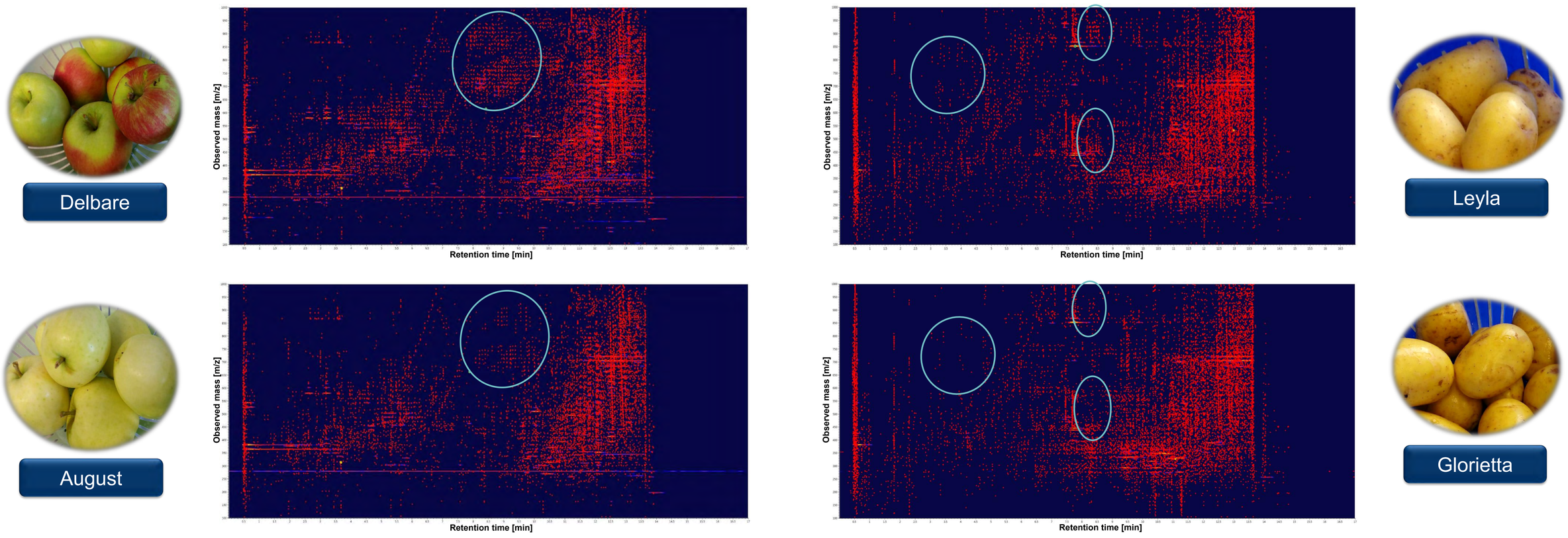


Fig. 1: The ion maps contain 10.000 MS peaks. The presented apple and potato varieties are from the same plantage or farm. A comparison of the patterns shows differences in the marked areas depending on the cultivar.

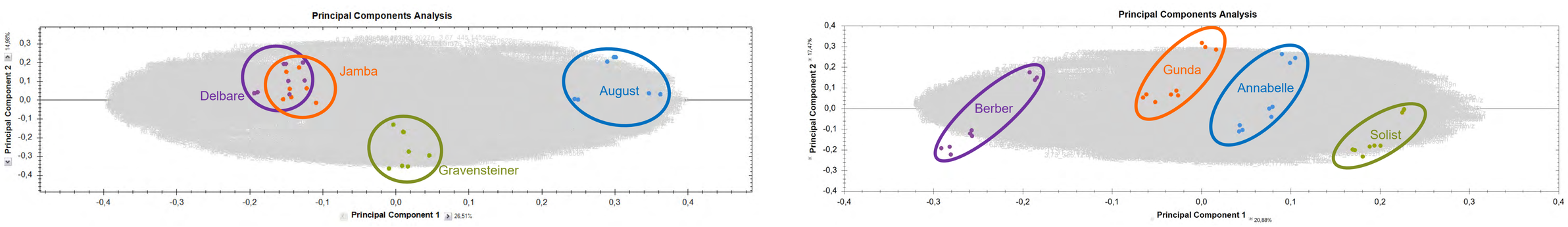


Fig. 2: Evaluation via PCA enables discrimination by botanical origin of apples (Delbare, Jamba, Gravensteiner, August) and potatoes (Berber, Gunda, Annabelle, Solist).

Perspective

The identification of selective marker substances and finally the establishment of metabolome databases and targeted methods using these marker compounds will pose future analytical challenges. Furthermore, influences of cultivation and seasonal conditions need to be eliminated considering samples from different harvest years. Additionally, predictive models to determine the botanical and geographical origin of potatoes and apples require model verification including blind samples.

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Metabolite analysis of the phenanthrene degrading, sulfate reducing bacterial enrichment culture (TRIP) using GC-MS

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Introduction (120/ 120)

Aerobic biodegradation of PAHs in the contaminated subsurface environment leads to swift depletion of dissolved oxygen and decrease of redox potential in these sites. Consequently, anaerobic biodegradation tends to get the dominant biodegradation process in the polluted subsurface. Despite of its importance, anaerobic biodegradation of PAHs has been poorly studied. The high complexity of the systems biology, matrix effect of culture medium compounds and disturbance of the secondary products (i.e.: bio-surfactants) makes the sample preparation and analysis a very challenging task in this field. The metabolite analysis of this study is aiming to enlighten the potential degradation pathway of phenanthrene under anaerobic, sulfate-reducing conditions, using TRIP enrichment culture. This culture is originated from samples of the Pitch Lake in Trinidad.

Experimental (75/ 120)

The aqueous phase of the culture was collected and sterile filtered after breaking of the bacterial cells. Metabolites were extracted using SPE cartridges (Bond Elut LCR-CN-E, 10 ml) and dichloromethane as solvent. Metabolites and reference standards were silylated prior to analyses using *N,O*-bis(Trimethylsilyl)trifluoroacetamide (BSTFA). Analyses were performed on an ISQ LT Single Quadrupol GC-MS-System with EI Ionization at 70 eV. Mass spectra were interpreted by matching to National Institute of Standards and Technology (NIST) database.

Results (207/ 300)

The metabolites observed in course of this study include phenanthrene carboxylic acid and its hydrogenated forms. This is an indicator that the degradation pathway of unsubstituted phenanthrene under anaerobic, sulfate reducing conditions is initiated by carboxylation of the non-substituted phenanthrene. This is in accordance with some of the results of the previous studies that reported anaerobic PAH degradation being initiated by carboxylation. The further degradation of phenanthrene carboxylic acid is expected to be continued with reduction of the aromatic ring. By comparison with the commercially available isomers phenanthrene-2-

carboxylic acid and phenanthrene-4-carboxylic acid, the metabolite present in the sample was identified as phenanthrene-2-carboxylic acid. This means bio-degradation of phenanthrene under anaerobic, sulfate reducing conditions is initiated in TRIP culture cells through substitution of the carboxyl group on the C-2 position of the aromatic ring.

A group of the observed byproducts of TRIP culture is bio-surfactants which are characterized to be from the fatty acids (namely: palmitic acid, stearic acid and arachidic acid). Presence of these bio-surfactants in the aqueous phase of TRIP enrichment culture was confirmed through a rapid drop-collapse assay.

Finally, the outcome of co-relation and comparison of different metabolites observed in this study was presented in a suggested anaerobic phenanthrene degradation pathway for TRIP enrichment culture.

New aspects (19/ 20)

Anaerobic phenanthrene bio-degradation pathway for TRIP culture under sulfate reducing conditions was suggested. Bio-surfactant production was observed as byproduct.

Key words

GC-MS, Metabolites, Anaerobic bio-degradation, Phenanthrene, TRIP

Real-time food authentication with a miniature mass spectrometer

Stefanie Gerbig, Stephan Neese, Alexander Penner, Bernhard Spengler, Sabine Schulz

Introduction

The number of food items in global trade is constantly increasing, and consequently the control of regulations regarding food adulteration has become increasingly important. From the analytical point of view, food authentication remains a challenging task, since the advancing performance of analytical methods and more sophisticated food fraud go hand in hand. Established mass spectrometric methods provide the opportunity to control food authenticity, including methods for marker detection as well as pattern analysis. [1,2] A portable mass spectrometer was utilized to record spectra since such analyses should ideally be carried out directly at the point of care. Data of metabolomic fingerprints of three different food groups were processed using principal component analysis (PCA).

Experimental part

A portable mass spectrometer (Mini 11) was utilized for fingerprinting food items. The instrument was developed by the group of Graham Cooks at Purdue University. [3] It consists of a linear ion trap providing unit mass resolution and a mass accuracy of 1-2 u. The measures of the Mini 11 are approx. 20x30x15 cm, its weight is 5 kg. Data was recorded in positive ion mode using electrospray, desorption electrospray and low temperature plasma ionization. The recorded raw data were processed with a home-built software called MSClassifier. This program employs principal component analysis (PCA) on spectra of known food items which can be stored in a repository and allows for spectra classification of unknown food items in real time.

Results and Discussion

Initial measurements comprised a set of three milk samples (goat milk, cow milk, soy milk). Approx. 200 mass spectra were recorded of each sample with ESI to enable statistical data analysis. Also, mixtures of cow and goat milk as well as cow and soy milk were prepared and spectra were recorded. This data was analyzed by PCA cross-validation and potential classifiers (Euclidean distance, mahalanobis distance and linear discriminant analysis) were tested. 99 % of the recorded single spectra of pure milk samples were classified correctly, the identification rate of milk mixtures was 94 % for cow and goat milk and 97.5 % for cow and soy milk mixture. Real-time analysis of new milk samples demonstrated the applicability of the statistical models for the identification of unknown samples.

Furthermore, low temperature plasma (LTP) was used for ionization to analyze different kinds of coffee beans. Single spectra of Arabica and Robusta coffee were recorded and subjected to statistical analysis. Results showed a high similarity of spectra, but nonetheless, a cross-validation experiment showed correct classification for 90% of robusta bean spectra and 96% for arabica bean spectra based on the coefficient of linear discriminant analysis. These measurements indicate that even low resolution and low mass accuracy data can be used for

pattern analysis and therefore aid in on-site identification of food items and the discovery of food fraud. After calculation of PCA models, real-time identification of coffee beans was successfully performed.
A third set of fish samples was analyzed using desorption electrospray ionization (DESI). Five different fish species were prepared for analysis by smearing a small piece of fish onto a glass slide and creating a thin film of tissue material. The spectra were again highly similar, but nonetheless the score plot of the PCA indicates separated group centers for each fish sample.

Novel aspects

Statistical analysis of data derived from miniature mass spectrometers allows for food authentication in real-time

Keywords

Miniature mass spectrometry, food analysis, authentication, principal component analysis

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Overview of imzML-based software tools for MS imaging

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imzML is **an open, vendor-neutral format for mass spectrometry imaging data**.[1] It provides more flexibility in data processing as the user is no longer limited to proprietary software but can choose the processing option that best fits the purpose. Measurement results (full data sets) can be shared between collaborators without loss of information (which is the case when sharing only the images). imzML is thus an important step towards more efficient collaboration as well as towards more transparent reporting of results in mass spectrometry imaging. Here we give an overview of available software tools which are compatible with imzML. All relevant information on imzML including technical specifications, available software tools and implementation examples is provided on the website ***www.imzml.org***.

Experimenteller Teil

The concept of imzML is **actively supported by the scientific community** and **major vendors of MS** imaging instrumentation (Thermo Fisher Scientific, Waters Corporation, IonTOF, Bruker Daltonik and Shimadzu). We give an overview of possibilities to convert MS imaging data to imzML. We also test the following **software tools that support imzML**, this includes open source (MSiReader by North Carolina State University, Omnispect by Georgia Institute of Technology, Cardinal by Purdue University and Northeastern University, SpectralAnalysis by Birmingham University), freely available (DataCubeExplorer by FOM-AMOLF, BioMap by Novartis, msiQuant by Uppsala University, SpectViewer by CEA, MSI.R by LabABI) and commercial (MALDIVision by Premier Biosoft) packages. Details and links for all software tools can be found on www.imzml.org.

Ergebnisse und Diskussion

imzML data can easily be stored, retrieved and analyzed with various available visualization tools. We are able to open and process imzML files in **12+ different software** tools. Each of them offers unique features which can be of help for specific applications. We give **a brief overview of functionalities** and also explain limitations/restrictions, e.g. some software tools are only able to process 'CONTINOUS' data. One important purpose of a common data format is to provide **flexibility in data processing and data sharing** between different labs. imzML data can be submitted to a **public data repository- PRIDE** database (www.ebi.ac.uk/pride/archive/) to make it publicly available to MS imaging community or to share with collaborators.[2] This will not only facilitate the realization of multi-laboratory collaborative research but also increase the reliability and transparency in the MS imaging field.Many tools are currently being developed or adapted to imzML. We also provide an outlook on these new upcoming tools. Most notably **imzML will be the input format for METASPACE** - a large European open source project for automated molecular annotation and identification in mass spectrometry imaging (metaspace.eu).

Neue Aspekte

imzML converters, Update on imzML based software tools, Comparison of visualization tools, Public repository for storage of MS imaging data

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Micro-arrays of faux tissue to investigate ion suppression effects in MALDI mass spectrometry of lipids

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MALDI mass spectrometry imaging (MSI) is increasingly used to visualize the molecular distribution of lipids and other biomolecules in tissue micro-sections. More recently, various QMALDI techniques were developed for quantitative imaging, typically by using internal standards. The largest complication in MALDI-MSI of lipids results from ion suppression effects.[1] To obtain a deeper insight into ion suppression phenomena under MSI conditions, fundamental studies are needed. However, natural tissue types and tissue homogenates, which are typically utilized for these studies, contain an extremely rich composition of different molecular constituents, which largely prohibit systematic studies. Here we developed artificial lipid-free "faux tissues" (FT) as substrates that enable a controlled adjustment of the lipid composition by spiking, while mimicking essential characteristics of soft tissue.

Experimenteller Teil

In order to measure FTs spiked with up to 24 different lipid compositions in one imaging run, a micro-array was constructed. Micro-array molds with vials of 2 mm in diameter and 5 mm depth, were filled with 20 µL of spiked FT material (please see results section below for details) and the block was then allowed to freeze at -18 °C. 20 µm-thick cryo-sections of the micro-array were prepared using a microtome and subsequently desiccated in a dry nitrogen atmosphere. For MALDI-MSI the sections were coated with 2,5-dihydroxybenzoic acid (DHB) matrix by using a sublimation/recrystallization protocol. MSI data were recorded with a QStar (AB Sciex) and a Synapt G2-S HDMS (Waters) mass spectrometer.[2]

Ergebnisse und Diskussion

A set of water-soluble polymeric substances that produce gel-like consistencies was tested as carrier for FT. These included gelatin, 2-hydroxyethyl cellulose (average Mv~1,300,000 g/mol), pectin, and carboxymethyl-cellulose (CMC) (average Mw~90,000 g/mol). Important criteria for their suitability to mimic soft biological tissue were their water content, texture, stiffness, handling of the material and its applicability for MALDI-MSI. Considering all factors, best results so far were obtained with CMC (3.3 %) for the carrier mold and a mixture of CMC and gelatin (both 2 %) as the FT material. All following experiments were, therefore, conducted with this combination of materials. We note that both materials are also widely used as embedding media for cryosectioning of tissue. Moreover, gelatin is a standard material to mimic biological tissue in a wide range of physical experiments (e.g., in nuclear physics and laser ablation experiments). In a next set of preparative experiments, the FT were spiked with different amounts of a phospholipid mix consisting of lipid concentrations in a range between 1 % and 6 % to generate tissues containing a lipid content comparable to brain tissue. After optimizing the matrix coating protocols for lipid analysis by using these preparations, we investigated the ion suppression effect of phosphatidylcholines (PC) on other phospholipid classes (e.g., phosphatidylglycerols (PG), phosphatidylethanolamines (PE) in pos. ion mode measurements) by varying the PC content of the FT and recording the ion signal intensities of all recorded lipid signals in dependence of the spiked lipid concentration.

Our preliminary results suggest that the employed „faux tissues“ form an easy to produce yet viable material to investigate basic mechanisms and fundamental problems in MALDI-MSI like ion suppression effects. In the future this could help to develop experimental protocols for a more reliable interpretation of MALDI-MSI data, an important step toward general quantitative imaging of lipids.

Neue Aspekte

Investigation of ion suppression effects in MALDI-MSI of phospholipids using novel artificial tissue material

Referenzen

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MALDI FT-ICR Imaging: Double the Performance or Double the Samples using Quadrupolar Detection

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For FT-based MALDI imaging, reducing the time to acquire each spectrum by milliseconds can shorten the total measurement time by hours. Quadrupolar detection (2ω) promises to dramatically enhance FTICR imaging studies by providing high MS performance with reduced transient length. In this study we evaluate the speed benefit of imaging with 2ω vs traditional 1ω and compare their MS performance.

Experimenteller Teil

Rat kidney and brain sections were coated with matrix using a pneumatic sprayer. 7T and 12T solarix systems were used, each fitted with a dynamically harmonized cell modified with new electronics that improves the 2ω signal intensities and allows fast switching between excitation and detection modes at the same electrodes. MALDI sensitivity was optimized for m/z 200-900 and images were collected. .

Ergebnisse und Diskussion

A major bottleneck for MALDI FT-ICR imaging is low sample throughput due to a compromise one must make between acquisition speed and high MS performance. With a small electronic change to a commercial system, one can achieve the same mass resolving power in half the acquisition time or 2x the mass resolving power from the same acquisition time. For example, with a 2s transient at 7T the 1ω signal produces a resolution of 300k at m/z 800 while the 2ω signal produces resolution of 300k with a 1s transient. The benefit for imaging studies is significant in that each measurement can be done in half the time without loss of mass accuracy or resolution. Alternatively, for the same acquisition time 2ω detection yields 2x the resolving power, 600k at m/z 800. Although no speed benefit is realized in this mode of operation there is benefit to resolving isotopic fine structure at higher m/z.

Neue Aspekte

2ω detection with MALDI FT-ICR doubles the resolving power or reducing the measurement time

Titel

Mass Spectrometry Imaging as Tool for the Analysis of MRI Contrast Agents in Biological Tissues

Introduction

The introduction of the first gadolinium-based contrast agent (GBCA) was followed by several other compounds which were quite similar from the safety, efficacy, bio distribution, mechanism of action, and pharmacokinetic point of view. Because of their high-stability these contrast agents were considered as safe and well-tolerated. However, more and more discussions about safety issues have been appeared in the last years. Imaging in mass spectrometry (MSI) stands for a powerful tool in investigation of distribution of drug compounds in biological tissue sections and thus, can provide exceptional insights into the fate of contrast agents in biological samples. The combined application of molecular and elemental mass spectrometry (MS) can complement each other and thus, confirm analytical results or even provide additional information.

Experimental Part

The tissues concerning various mice organs were stored in the freezer at -80 °C. Initially, these tissues were cryo-sectioned using a cryotome, thaw-mounted onto microscope glass slides and dried under vacuum atmosphere in a desiccator. The samples were covered with DHB matrix applying an airbrush. Subsequently, MALDI-MSI measurements were performed. Afterwards, these tissue sections measured by MALDI-MSI were printed with a Ho spiked ink used as internal standard (IS) and LA-ICP-MSI measurements were implemented. Finally, software based analysis and image construction were executed.

Results and Discussions

This work includes a strategy to detect and localize gadolinium-based contrast agents (GBCA) in biological and medical relevant samples implementing mass spectrometry imaging (MSI) techniques in particular matrix-assisted laser desorption ionization mass spectrometry imaging (MALDI-MSI) as well as laser ablation inductively coupled plasma mass spectrometry imaging (LA-ICP-MSI). Sample preparation was performed prudently to sustain localization of these highly hydrophilic GBCA and keep spatial information of the respective tissue sample. Matrix application was decided to perform manually using an airbrush in a constant set-up leading to reproducible results. In this way, distinct GBCA could be detected and localized in various kinds of tissue samples using high resolution MALDI-MSI. The resulting data was normalized by commonly applied methods, e.g. deviation through certain mass-to-charge ratio (*m/z*). The samples analyzed by MALDI-MSI were also measured using LA-ICP-MSI. Due to fluctuations and instrumental drifts during long time measurements a matrix matched

internal standard (IS) was introduced. In conclusion, both methods MALDI- and LA-ICP-MSI are in good agreement. LA-ICP-MS as elemental MS technique could confirm the results obtained by molecular MS.

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New Aspects

Complementary of molecular and elemental MSI could be demonstrated concerning GBCA in biological tissue sections.

Keywords

MRI contrast agents, mass spectrometry imaging, biological tissues

Optimized Biomolecular Extraction Using Desorption by Impulsive Vibrational Excitation: Applications to Embryonic Cell Differentiation

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The sensitivity of mass spectrometry is ever approaching the fundamental limit of single molecule detection. Picosecond Infrared Laser (PIRL) based Desorption by Impulsive Vibrational Excitation (DIVE)[1] has provided significant advantages for on-the-fly mass spectrometry analysis on both native and denatured protein systems, opening new fields of application, e.g. in single-cell analysis and enhanced surgical biopsies. The possibility of obtaining spatial information on the distribution of proteins in cells promises new insights into the process of cell differentiation during embryonic development. Here we develop a DIVE ablation based extraction and optimized plume collection system for both aqueous solutions as well as tissue samples.

Experimenteller Teil

The system is based on previously described droplet capture surface sampling methods utilizing UV and visible lasers.[3] The beam of a PIRL operating at a wavelength of 3 µm is focused onto the surface of the sample mounted on a multi-axis translation stage. The resulting ablation plume is captured into a droplet of buffering solution suspended approximately 0.5 mm above the sample. Alignment and optimization of the setup is performed using two long working distance microscopes. The capture buffer is optimized for specific analytes, typically containing reagents that maintain a constant pH and prevent proteolysis and the elimination of phosphate moieties. Captured analytes were analyzed using a Bruker ion-trap MS operating in ESI mode.

Ergebnisse und Diskussion

Ablation of biomaterial via DIVE employs a picosecond IR laser, immediately exciting the O-H stretch vibration of H2O to drive water molecules into the gas phase on an ultrafast timescale.[2] The process occurs faster than thermal and acoustic energy relaxation to the surrounding tissue, yet the laser pulse is long enough to avoid the unfavorable effects of multi-photon ionization and plasma formation. Hence, molecules included in the sample are softly transferred into the gas phase leaving large biomolecules, such as proteins, intact and undamaged. The method provides efficient extraction of species ranging from small molecules to large MDa complexes and even entire viruses.

Recent experiments have shown that tissue homogenization by DIVE ablation leads to increased protein species identification from samples (human tonsil) compared to conventional homogenization techniques.[1] Furthermore, the method preserves macromolecules by reducing the degree of fragmentation.[5] The ultrafast nature of the extraction results in a reduced degree of proteolysis for extracted protein species, creating a more accurate picture of the true proteome of native cells. Here we develop and characterize direct droplet capture of the DIVE ablation plume for soft extraction, transfer and collection of peptides, proteins and macroscopic protein crystals. The method will be applied to significantly increase the detectability of low abundance proteins in mesenchymal cells and

allow insights into the mechanism behind cell differentiation in embryonic development using *Danio rerio*[4] as a model organism. For an in-depth investigation of the method's capabilities MS-assisted proteome analysis results will be compared for two cell lines, namely HEK-293 and U2OS, both on homogenates obtained by various cell lysis methods and on native tissues sampled by DIVE-ablation. The method is expected to be further applicable to the field of biodiagnostics, e.g. allowing distinction of healthy cells from those affected by cancer during the course of surgical tumor resection.

Neue Aspekte

Droplet collected DIVE biomolecular extraction allows soft extraction of fragile molecular species with high collection efficiency and minimal molecular degradation.

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Development of Sub-Cellular Mass Spectrometry Imaging by Impulsive IR Laser Ablation

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Improving upon the concept of matrix assisted laser desorption ionization with ultraviolet light (UV-MALDI), infrared laser desorption ionization (IR-LDI) reduces fragmentation and is capable of analyzing water rich samples without the requirement for an often detrimental matrix by targeting the O-H stretching vibration of water for efficient energy deposition and ablation. Employment of an IR laser source in the picosecond regime, recently demonstrated by our group [1-2] as desorption by impulsive vibrational excitation (DIVE), allows for the ablation event to occur under thermal and stress confinement conditions. This minimizes damage to surrounding sample areas, reduces the laser fluence necessary for ablation, and decreases the time molecules spend in the initial, dense ablation plume where most fragmentation takes place.

Experimenteller Teil

We have developed a reflectron time-of-flight (TOF) mass spectrometer with a custom designed, high vacuum cryogenic sample transfer system and in-vacuum DIVE ion source to characterize the new ultra-soft ablation technique with minimal interference from ambient gas pressure. In order to extend the spatial resolution of IR-LDI imaging mass spectrometry [3] to the cellular level, we design an ion-microscope-coupled DIVE-TOF system. Complementary characterization of the ablation plume expansion was performed via time-resolved interference microscopy using a home built setup. The method is sensitive to minute changes in the index of refraction and therefore capable of determining the particle velocity and directionality even for small amounts of desorbed gas phase water and provides information about the ablation mechanism and plume dynamics.

Ergebnisse und Diskussion

Experimental [4] as well as computational [5] studies have shown DIVE ablation to be an efficient means of extracting and ionizing even large molecules with minimized collisional fragmentation. The picosecond infrared laser (PIRL) employed here produces pulses with durations of only 10ps and accordingly uses comparably low output powers, enabling for the first time a systematic study of laser ablation at the lower end of the DIVE regime. We demonstrate the functionality of the ion source and mass spectrometer showing first spectra. Characterization of the ejecta's axial velocity distribution and the ablation event progression over time - i.e. the onset of desorption, recoil ejection, etc. – is necessary for optimizing the spatial and mass resolution of the TOF-MS system, and is provided by interference microscopy measurements. The lateral velocity distribution is of specific significance for mass spectrometry imaging.

Neue Aspekte

Interfacing a PIRL-based ion source with an ion microscope mass spectrometer promises to unveil the proteomic map of the cell.

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Towards qMALDI-MSI : MS imaging of phospholipids in mouse cerebellum followed by semi-quantitative nano-HPLC-ESI-MS of extracts from laser micro-dissected brain regions

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MALDI-MS imaging is increasingly used to record the distribution of phospho (PL-) and further lipids in microsections of animal and plant tissues. However, because of potentially varying extraction efficiencies within different tissue regions, and ion suppression effects in mixtures, there is a notable risk that the MALDI-MSI-derived ion images may not even correctly reflect the relative abundances of a specific compound [1]. The aim of this work was to study the effect of factors such as the biological matrix on the MALDI-MSI ion yields and to thereby identify strategies for improved quantitative MALDI-MSI. We used a combination of MALDI-MSI of mouse cerebellum sections and laser micro-dissection (LMD) of hereby identified brain regions. Semi-quantitative analyses were achieved using nano-HPLC-ESI-MS of extracts.

Experimenteller Teil

16 µm-thick cryo-sections were thaw-mounted on laser-microdissection slides (Zeiss). Tissue coating with 2,5-dihydroxybencoic acid matrix was achieved with a sublimation/recrystallization protocol [2]. Synapt G2-S instruments (Waters) was used for all MS runs. Both conventional MALDI-MSI [3] and postionization-laser-based MALDI-2-MSI [2] experiments were performed. A focal laser spot of ~10 µm in diameter and a pitch size of 50 µm were used. In this “undersampling mode”, the largest fraction of the tissue sections was not interrogated by the laser beam. Based on the MSI data, ROIs were identified, micro-dissected, and transferred into individual vials by use of a PALM system (Zeiss). Lipids were extracted using methanol/methyl tert-butyl ether (1:3, v/v) and separated with a nano-HPLC system (Ultimate-3000, Thermo Fisher Scientific).

Ergebnisse und Diskussion

We successfully established MALDI-MS imaging of the brain sections and the subsequent laser-microdissection of regions identified in the MALDI images directly from a single PALM laser-micro-dissection slide.PLs from the cut regions were micro-extracted using the methanol/methyl tert-butyl ether-based protocol. Use of the nano-HPLC with a C18 column (75µm x 150mm) provided fractionation of lipids. Background ions derived from the transfer membrane were not detected within the relevant elution time window. Due to extraction and the chromatographic separation step, the lipid content of the different regions of mouse cerebellum could be analyzed independent of its biological matrix, (i.e., without interferences by ion suppressing constituents). Comparison of the ESI-MS results from HPLC-separated extracts as obtained from different brain regions (e.g. the white versus gray matter) with the MALDI-MSI data obtained from the same areas allowed a first characterization of possible interdependences of lipid species and apparent suppression effects. This way a first rough correction of MALDI-MSI data for evidently suppressed lipid species could be performed. For example the signal ratio of a PC and a PG species varies greatly between the MALDI-MSI and HPLC-ESI-MS measurement. Based on the primary findings, our next steps will

encompass establishing total quantification using internal standards and different columns (HILIC, NP) that will be incorporated into the HPLC-ESI-MS work flow.

Neue Aspekte

Complementary measurement of the phospholipid content in mouse cerebellum by MALDI-MSI and nano-HPLC-ESI-MS of laser micro-dissected areas.

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A new internal standard approach for laser ablation ICP-MS of polyacrylamide gels

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Introduction

Laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) in bio analysis has proven to be a versatile technique providing images with both high sensitivity and spatial resolution.[1] One potential application is the quantification of element-containing or labelled proteins separated with gel electrophoresis directly from the gel. However, one challenge that still needs to be solved is the normalization and calibration of the signal to account for plasma fluctuations or inhomogeneities of the ablated surface. Up until now, normalization is based either on using the 13C isotope signal[2] or thin layers of elements applied as standard on top of the gel.[3,4] However, both approaches are limited by several disadvantages. Here, we present a new approach for internal calibration, incorporating elemental standards into the gel matrix.

Experimental section

A stable complex of the metal used as internal standard is incorporated covalently into the gel matrix of polyacrylamide gels. Mixtures of defined ratios of standard proteins bovine serum albumin and α-lactalbumine are labelled with MeCAT[5] and subsequently separated with gel electrophoresis. Gels can be processed as usual, including staining with Coomassie brilliant blue. Protein bands are excised, dried and then analysed by LA-ICP-MS. Laser ablation is performed with aUP213 Laser ablation system using a SuperCell^{Tm} (Nd:YAG, New Wave Research, Inc.) coupled to an Element XR ICP-MS (Thermo Fisher Scientific). Images are generated using Origin software (OriginPro 9.1G).

Results and discussion

As internal standards mainly lanthanide ions were used, due to their high sensitivity and few interferences in ICP-MS. Homogeneous distribution of the standard inside the gel could be verified both by LA-ICP-MS and direct infusion ICP-MS of mineralized gel spots. Normalization significantly increased the quality of the images especially regarding local deterioration of the laser focus when measuring large areas and regarding comparability of different measurements also on different days. Therefore, with normalization protein ratios of different measurements corresponded much better with the theoretical ratios. Moreover, by using elements that are not biologically available as internal standards, even unintentional surface contaminations during the processing, e.g. from dust, will not falsify the normalization, which can be a problem when using ^{13}C for normalization. Since the standard is distributed inside the gel matrix in comparison to the thin layer approach, where it is on top of the gel, the method also considers inhomogeneities of the surface structure like crates or air bubbles. Although high spatial resolution is often not required when assessing gel surfaces, it is nevertheless often limited by crystal size and shape when using the thin layer approach. Ultimately the new method has the potential to use the internal standard for absolute quantification of the proteins inside the gel, which will be addressed in the near future.

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Multimodal imaging combining mass spectrometry and vibrational spectroscopy using a single tissue section and an integrated data processing workflow

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Introduction

Multimodal imaging is a powerful tool to compensate the limitations of individual imaging techniques in order to obtain a better understanding of the chemical composition of (biological) samples. Mass spectrometry provides a detailed insight into the chemical composition of biological tissue while vibrational spectroscopy yields quantifiable information about protein and lipid content. In addition, Fourier-transform infrared (FT-IR) provides very fast acquisition. In this work, a workflow has been developed in which atmospheric pressure matrix assisted laser desorption/ionization mass spectrometry (AP-MALDI-MS), Fourier-transform infrared (FT-IR) and Raman spectroscopy are applied to analyze a single tissue section. All data is combined in an integrated processing workflow (based on the open data format imzML).

Experimental

FT-IR images were performed on a mouse brain tissue section using an infrared microscope (Hyperion 3000, Bruker Optik), wavenumber range was 3400-1250 cm^{-1}. For Raman imaging a LabRam HR800 (HORIBA Jobin-Yvo) equipped with a 532 nm laser and a 50x objective was used (10 µm pixel size, integration time 2x2.5s). Subsequently dihydroxybenzoic acid (DHB) was applied on the same section. MSI analyses with 10 µm spatial resolution were performed using the AP-MALDI source (TransMIT, Giessen, Germany) coupled to an Q Exactive HF (Thermo Fischer Scientific) in the lipid mass range (*m/z* 700-900). Finally, the tissue section was stained with HE. After conversion to imzML, the visualization of the data was performed using the open-source software MSiReader.

Results

The presented workflow for multimodal imaging consists of 5 steps which are performed on the same tissue section: FT-IR measurements, Raman measurements, matrix application, AP-MALDI-MS measurements and HE-staining.

As no software existed to process Raman and MS data simultaneously, a LabView program was developed to convert Raman and FTIR data to imzML. This provides more flexibility in data processing as the user is no longer limited to proprietary software. It also allows to use the same settings for the visualization of Raman (or any spectral) and MS data. The conversion tool is not limited to spectroscopic data, but can be applied to any ASCII formatted data that was acquired in spatially defined manner.

FT-IR, Raman and MS images allowed for discrimination between gray and white matter. Purkinje cells could be clearly identified in the MS, but less clearly in the Raman images. As the Raman spectra were acquired in the fingerprint wavenumber range (400-1800cm^{-1}), the discrimination is mainly based on protein, lipid and heme content. Due to Resonance Raman scattering, two heme species, cytochrome c and heme from dried blood could be differentiated. FT-IR provides a rapid overview about lipid and protein composition of the whole section. This helps to define the areas of the tissue sections to be measured with Raman and MS as these usually require significantly longer acquisition times (per pixel). AP-MALDI-MS spectra were acquired with high mass accuracy (< 2ppm) and high mass resolution (240,000) in positive ion mode and provide information about the distribution of phospho- and sphingolipids.

As spectroscopic, MS and histological images showed very high correlation of structural features, the developed workflow was shown to be feasible and robust. The proposed workflow is flexible and can be adopted to additional/alternative imaging techniques such as Atomic Force Microscopy (AFM) and Coherent Anti-Stokes Raman Spectroscopy (CARS).

Localization of Ergot Alkaloids in Sclerotia of Claviceps purpurea by MALDI-MS Imaging

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The fungus *Claviceps purpurea* produces highly toxic ergot alkaloids and accumulates these in the hardened bodies of fungal mycelium, called sclerotia [1]. The sclerotia replace the crop seed of infected grass species and are known to infect more than 400 different grass species, which include numerous important food- and feedstuff such as wheat and rye. Ergot alkaloids pose a serious public health threat. While several studies have explored details of the development of the ergot bodies, little information is available on the spatial distribution of the mycotoxins in the sclerotia. Here we show, at the example of two representative alkaloids, ergocristine and ergometrine, that MALDI-MSI constitutes a powerful tool for visualization the distribution of the mycotoxins at ten micrometer resolution.

Experimenteller Teil

Male sterile rye plants (*Secale cereale*) were infected with ergocristine and ergometrine-producing *Claviceps purpurea* strains Ecc93 and Gal 310, respectively. 24 days post inoculation the sclerotia were harvested and shock frozen in lq. N_2. 15 µm-thick cryosections were spray-coated with 2,5-dihydroxybenzoic acid matrix. We employed a modified Synapt G2-S HDMS mass spectrometer (Waters), enabling MALDI MS imaging (MSI) experiments with a focal laser spot size of ~10 µm in diameter and operation at an elevated N_2 pressure of ~1 mbar in the ion source [2].

Ergebnisse und Diskussion

A first crucial prerequisite for the experiments was the development of a suitable embedding protocol. To obtain intact 15 µm-thick cryosections from the fragile sclerotia, consisting of a hardened outer shell and a fat-rich soft inner part, we embedded them in a mixture of 2% 2-hydroxyethyl cellulose and 2% carboxymethyl cellulose (*w/v*) polymers and developed an easy to handle mounting protocol. To minimize ion suppression effects, tissue sections were furthermore degreased with chloroform prior to matrix coating.

Using MALDI-MSI, ergocristine was detected as $[M+H]^+$, $[M+Na]^+$ and $[M+K]^+$ ion species, whereas, due to its higher polarity, ergometrine was detected predominantly as $[M+H]^+$ ions. Characteristic in-source decay fragments together with MS/MS-spectra recorded from tissue and by HPLC-ESI-MS from extracts and standards unequivocally confirmed the molecular identities. In contrast to the successful MSI measurements conducted with the Synapt, intact molecular ions of the alkaloids were not obtained upon use of an axial-TOF-instrument. We attribute this finding to the necessary stabilization of the labile molecules by collisional cooling.

The MALDI-MSI experiments (performed at 35 µm pitch size) revealed that ergocristine was enriched in the proximal region of the Ecc93-derived sclerotia and that the toxin concentration increased from the rim to the center. Notably, no ergocristine signals were detected in the

sphacelial cap nor in the sphacelial region in the embraced residue in the center. Thus, ergocristine was mainly concentrated in the base of the sclerotia. In contrast, ergometrine was more evenly distributed throughout the smaller Gal 310-derived sclerotia, with only a slight enrichment in the proximal region.

Our data show that MALDI-MSI constitutes a useful complimentary technique for studying the development of ergot bodies and for determination of alkaloid distributions. Additional information is available in ref. [3].

Neue Aspekte

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CoolMALDI: Combination of IR-ablation and UV-postionization of snap-frozen tissue sections for sensitive imaging of lipids and metabolites

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UV-MALDI-MS imaging of metabolites is hampered by a possible overlap of the ion signals with matrix-derived background ions and, by breaking the cool chain, metabolic turnover processes might alter the initial molecular landscape. Here we developed a cooling stage for a MALDI-2 Synapt G2-S HMDS mass spectrometer (Waters) [1] preserving samples at cryogenic temperatures. This way endogenous tissue water can be used as matrix for IR-MALDI-MSI of snap-frozen samples. To enhance ion yields, it was combined with UV-postionization similar to MALDI-2 [1]. Next to describing the technical principle and examining crucial physical parameters, we will show first MSI results indicating a large potential of this novel method for the analysis of physiologically relevant metabolites as well as phospho- and glycolipids.

Experimenteller Teil

Using a continuous flow system based on lq. N_2 as cooling medium and a counter heating unit enabled adjustment of the target temperature (T) within +100 and -180 °C. Typically, T was fixed at -100±1 °C during MSI runs and the N_2 buffer gas pressure set to ~1 mbar. An infrared optical parametric oscillator (IR-OPO) laser (alphaScan, GWU Lasertechnik; l=2.94 µm; t=7 ns; E_{pulse}~4.5 mJ) served for material ablation. The focal spot size was ~100 µm x 70 µm. An UV-OPO (versaScan, GWU; λ=220-320 nm; t=7 ns; E_{pulse}³600 µJ) served for postionization. The UV-laser beam had a focal diameter of ~100 µm and was intercepting the IR-laser generated particle plume orthogonally at a distance of ~500 µm.

Ergebnisse und Diskussion

Fundamental studies investigating the effect of postionization laser wavelength, delay between the two laser pulses, buffer gas pressure, and sample temperature were conducted with homogenized pig brain tissue, providing a uniform ion response across the whole 10 mm x 50 mm-wide sections. These studies revealed that PI yields strongly depend on buffer gas pressure, delay between IR and UV-laser pulses and the interplay of UV-laser wavelength and absorption characteristics of the analytes. Furthermore the thickness of the tissue sections seems to have an influence.

MALDI-MSI data acquisition from 15 µm-thick mouse brain sections was achieved at a pitch size of 75 µm x 75 µm. The obtained mass spectra were exceedingly rich and included molecular ion signals of metabolites from a wide range of molecular classes including polar and lipo-soluble metabolites (e.g., amino acids, free fatty acids, vitamins and classical neurotransmitters). Compared to the single laser IR-MALDI mode, the use of the additional UV-laser boosted ion signals by up to 3 orders of magnitude. Moreover, numerous phospho- and glycolipid species were detected in parallel. We propose that the underlying mechanisms comprise both direct 2-photon ionization of resonantly absorbing molecules at the primarily used 260 nm-wavelength and indirect charge transfer processes taking place in the particle plume. Examples of coolMALDI images of physiologically relevant metabolites visualizing characteristic mouse brain structures will be presented.

Neue Aspekte

New coolMALDI method for matrix-free MSI of metabolites and lipids from snap-frozen samples

Referenzen

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Application of the Superbasic Matrix DPN in Atmospheric Pressure MALDI-MS-Analyses of Biological Samples

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Introduction:

Matrix-assisted laser desorption/ionization mass spectrometry (MALDI-MS) of small molecules requires special matrices, which do not generate interfering signals below 500 *m/z*. The recently introduced superbasic matrix 1,8-di(piperidinyl)naphthalene (DPN), fulfills this requirement and features superior ionization properties, which result in higher signal intensity in negative ion mode than previously reported ionless matrices**[1]**. Here, we like to demonstrate the benefits of using DPN in AP-MALDI analyses of various biological relevant samples. Especially AP-MALDI-MS-imaging experiment profited from the higher sensitivity as smaller spot sizes and therefore a higher spatial resolution can be achieved.

Experimental:

1. AP-MALDI-FTMS analysis of whole blood:
   Fresh human blood was diluted with deionized water, mixed with a DPN-solution and spotted on an AP-MALDI-target plate. After drying of the plate, the spots were analyzed in negative ion mode using an AP-MALDI-PDF+ ion source coupled to an orbitrap mass spectrometer.

2. AP-SMALDI-FT MSI analysis of *Drosophila melanogaster*:
   Intact *Drosophila* flies were embedded in O.C.T. medium and cut into sections with a thickness of 25 µm. The dry sections were covered with DPN matrix by sublimation and imaged with a step size of 15 µm.

3. AP-SMALDI-FT MSI analysis of *Arabidopsis thaliana* leaves:
   Intact and mechanically wounded leaves of *A. thaliana* were covered with DPN, fixed on a glass slide, dried and scanned with a step size of 50 µm.

Results and discussion:

1. AP-MALDI-FTMS analysis of human blood:
   The analysis of human blood with AP-MALDI MS in combination with DPN-matrix yielded rich spectra of almost 200 metabolites within only few minutes after sampling with minimal sample preparation. The obtained signals are derived from amino acids, fatty acids, various small peptides, various forms of heme B as well as lysed and intact phospholipids. The identities of the metabolites are based on accurate mass data and were further supported using CID experiments. Using labeled internal standards free fatty acids were quantified. These results show that our method could help to provide detailed and fast information about the metabolic composition of various complex biological fluids without any need for complicated sample preparation and/or extraction procedures.

2. AP-SMALDI-FT MSI analysis of *Drosophila melanogaster*:
   The common fruit fly *Drosophila melanogaster* is one of the major model organisms for genetic and metabolic studies, which would greatly benefit from the ability to localize and identify specific metabolites within the insect. It was demonstrated that MALDI-MS imaging can be effectively used to localize lipid species of several classes in sections of *D. melanogaster***[2]**. These studies however focus predominantly on positive ion mode and therefore cover only a part of the analyzable metabolome. In our AP-MALDI-MSI experiments with DPN we used the negative ion mode and obtained ion maps of several lipid species as well as small metabolites like glucose and glutamic acid. These maps were detailed enough to allow the profiling of individual organs within the fruit fly.

3. AP-SMALDI-FT MSI analysis of *Arabidopsis thaliana* leaves:
   To study the release of defense and stress related metabolites, leaves of *A. thaliana* were analyzed using AP-SMALDI-FT MSI with DPN as matrix. Several ion maps of stress related glucosinolates could be obtained from intact and mechanically wounded leaves.

Novel aspects:

Improved sensitivity for neg. mode AP-MALDI-MS-imaging of biological samples.
Fast detection and identification of metabolites in blood via AP-MALDI-FT-MS with DPN-matrix.

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Keywords:

Superbasic matrix DPN, AP-MALDI, AP-SMALDI-FT MSI, lipids, glucosinolates

Collision Specific Fragmentation of Oligonucleotides in Tandem Mass Spectrometry Experiments

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Keywords Collision induced dissociation (CID) · Higher energy collision dissociation (HCD)· Mass spectrometry · Oligonucleotide Fragmentation

Introduction

MS/MS experiments prove extremely useful for identification and quantification especially in complex mixtures. In collisional dissociation tandem MS a precursor ion is isolated before it is exposed to a multitude of controlled inelastic collisions with neutral atoms or molecules resulting in high internal excitation into a dissociative state. Technically, HCD uses a higher individual collision energy, while CID relies on a larger number of collisions [1]. Since peptide fragmentation via CID and HCD results in almost identical fragmentation pattern the techniques are often falsely used synonymously. We present here the different results obtained by CID and HCD for DNA which is known from photodissociation studies to undergo highly specific dissociation behavior [2,3].

Experimental

All oligonucleotides (ACTG, CTGA, TGAC, GACT, AAAA, TTTT, CCCC, GGGG) were analyzed at a final concentration of 10 µM in water with 30 % methanol and 1 % triethylamine. Negative ion ESI-MS spectra were obtained with a LTQ Orbitrap XL. Parameters were as follows: 100 °C transfer capillary temperature and 30 arbitrary units as sheath gas flow (nitrogen). Samples were directly infused at 10 µL/min for MS experiments. The precursor ions were isolated for CID and HCD experiments with an isolation width of Δ m/z 2 and fragmented with an activation time of 30 ms, while the relative collision energy was varied between 0 % and 100 % in steps of 1 %.

Results

This study compares the fragmentation of oligonucleotides of various sequences with two different MS/MS methods commonly used in Omics research. In total eight 4-mer oligonucleotides were measured with both CID and HCD fragmentation. The minimum activation energy necessary for complete fragmentation for each of the eight individual precursor ions was determined allowing a comparison of the resulting spectra. In contrast to peptides, the spectra showed a pronounced collisional specificity in their distribution of fragments. The comparison of CID and HCD reveals a fundamental difference in fragmentation dynamics. While the total number of fragments itself is almost similar, the nature of the fragments, i.e. the site where the bond break occurs, differs. For example the negative base loss channel is significantly favored in HCD, while CID favors $[M-H_x-B]^{x-}$ fragmentation as a dominant channel (Fig.1).

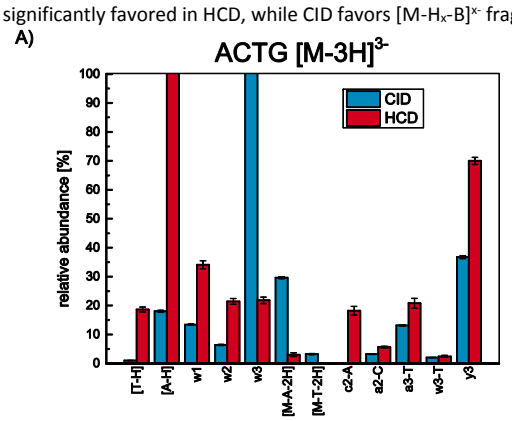

Fig 1. *Relative abundances for all observed fragments in the spectra of the three-fold negatively charged 4-mer ACTG. Intensities of CID experiments are in blue, and of HCD experiments in red.*

Both methods use collision dissociation with neutral atoms or molecules and are often treated equally. Our results proof the need of comparison using MS/MS experiments of new uncommon samples, because it seems to be hardly foreseeable if there is or is not a difference in fragmentation. This also establishes the accessibility of additional information out of MS/MS results due to the potentially complementary character of CID and HCD Tandem MS methods, respectively.

New Aspects

The results show the need to treat HCD as an additional sometimes complimentary method rather than an equivalent substitute.

Literature

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REMPI- und MATI-Spektroskopie an den Methylpyridinen

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Einleitung (119/120)

Pyridin ist ein Grundgerüst von vielen biologisch relevanten Molekülen, wie Nikotin und Vitamin B_3. Biochemische Prozesse beruhen oft auf elektrostatischen Wechselwirkungen zwischen Molekülen, die durch die elektronische und geometrische Struktur der Verbindungen definiert werden. Die Charakterisierung der Elektronenverteilung und geometrischen Verhältnisse in unterschiedlichen elektronischen Zuständen kann über die *Resonant-Enhanced-Multi-Photon-Ionization* (REMPI)- und in ionischen Zuständen über die *Mass-Analyzed-Threshold-Ionization* (MATI)-Spektroskopie erhalten werden.

Das Pyridin wurde umfangreich mittels REMPI- und MATI-Spektroskopie untersucht und charakterisiert [1]. Die Methylpyridine wurden hingegen bis zum jetzigen Zeitpunkt hauptsächlich absorptions- und photoelektronenspektroskopisch vermessen. Die Charakterisierung des S_1 ($n \rightarrow \pi^*$)- und D_0-Zustandes war das Ziel dieser Arbeit. Insbesondere der Unterschied zwischen 2- und 3-Picolin, die eine C_s-Symmetrie aufweisen, zum 4-Picolin mit einer C_{2v}-Symmetrie war aufgrund unterschiedlicher Symmetrien sehr interessant.

Experimenteller Teil (112/120)

Die Methylpyridine wurden mittels REMPI- und MATI-Spektroskopie untersucht. Die Messungen wurden mit zwei Farbstofflasern der Firmen *Laser Analytical Systems* und *Lambda Physics* und einem Eigenbau-Flugzeitmassenspektrometer durchgeführt.

Die Analyten wurden durch eine gepulste Jetdüse ins Vakuum überführt. Bei der REMPI-Spektroskopie erfolgte anschließend eine elektronische Anregung durch den ersten und die Ionisation durch den zweiten Laser. Zur Aufnahme der REMPI-Spektren wurde der erste Farbstofflaser spektral durchgestimmt. Für die Messung der MATI-Spektren wurde der erste Farbstofflaser resonant auf einen vibronischen Übergang eingestellt und der zweite Laser durchgestimmt. Die Separation der prompt gebildeten Ionen von den Rydberg-Neutralen erfolgte durch ein Bremsfeld. Nach wenigen Mikrosekunden wurden die Rydberg-Moleküle durch einen HV-Puls feldionisiert und auf einen MCP-Detektor beschleunigt.

Ergebnisse und Diskussion (217/300)

Die Anregungsenergien des ersten elektronisch angeregten Zustandes (S_1) wurde bei 2-Picolin zu 34766 ± 3 cm^{-1} (4.3014 ± 0.0004 eV), bei 3-Picolin zu 34660 ± 3 cm^{-1} (4.2973 ± 0.0004 eV) und für 4-Picolin zu 35177 ± 4 cm^{-1} (4.3614 ± 0.0005 eV) bestimmt. Die REMPI-Spektren vom 2- und 3-Picolin unterschieden sich hinsichtlich Anzahl der aktiven Banden deutlich von dem REMPI-Spektrum des 4-Picolins. Im REMPI-Spektrum des 4-Picolins waren deutlich mehr Banden aktiv, was durch einen Symmetriebruch bei der elektronischen Anregung bedingt war. Alle drei Methylpyridine erfahren bei der elektronischen Anregung in den S_1-Zustand eine Geometrieveränderung entlang des Eigenvektors der Mode 6a. Im 4-Picolin hat zusätzlich eine der 6a ähnliche Schwingung einen signifikanten Beitrag am elektronischen Übergang.

Die adiabatischen Ionisationsenergien des 2-, 3- und 4-Picolins wurden zu 72371 ± 5 cm^{-1} (8.9729 ± 0.0006 eV), 72613 ± 5 cm^{-1} (9.0026 ± 0.0006 eV) und 72932 ± 4 cm^{-1} (9.0424 ± 0.0005 eV) bestimmt. Die drei Methylpyridine zeigen bei der Ionisation aus dem S_1-Zustand eine Geometrieverzerrung entlang des Eigenvektors der Schwingung 8b. Im MATI-Spektrum über den elektronischen Ursprung im S_1-Zustand des 4-Picolins weist außerdem die Methyltorsion eine sehr hohe Intensität auf. Sie wirkt als falscher Ursprung in diesem Spektrum. Der Charakter des falschen Ursprungs kann auch für die Mode 6a im MATI-Spektrum über die Schwingung 6a im S_1-Zustand des 2-Picolins beobachtet werden.

Neue Aspekte (20/20)

Die adiabatischen Ionisationsenergien der Methylpyridine wurden hochgenau bestimmt und die geometrischen Veränderungen bei der elektronischen Anregung und der Ionisation charakterisiert.

Literatur (1/5)

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Stichworte (5/5)

Pyridinderivate, REMPI-Spektroskopie, MATI-Spektroskopie, Anregungsenergien, Ionisationsenergien

Ultra High Throughput Drug Discovery Screening by MALDI-TOF Mass Spectrometry

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Mass Spectrometry (MS) is a powerful technique for studying biomolecules and is particularly useful for screening large molecular libraries. As a direct analysis, label free technology, MS enables assays to be generated that monitor native analytes, in contrast to commonly used fluorescent or colorimetric techniques that require modifications to analytes that may perturb native pharmacology. Traditionally MS based techniques have been relatively slow and thus not suited for high throughput screening (HTS – 10,000 compounds/day) or ultra HTS (uHTS – 100,000 compounds/day).

Matrix-Assisted Laser Desorption/ Ionization time-of-flight (MALDI-TOF) MS provides an alternative format for HTS/uHTS of small molecules, peptides and proteins for enzyme assays.

Experimenteller Teil

With analysis times ~1 second/sample and nanolitre volumes, this technique offers a MS format with throughput and sample volumes closer to traditional HTS/uHTS fluorescence based technologies but with a label-free, direct-detection assessment of activity.Here we describe the development and validation of assays using MALDI-TOF coupled to nanolitre liquid handling for HTS and uHTS. Exploiting the speed and accuracy of the Cybi®-well VARIO pipettor with
1536 air displacement ceramic pistons and the next generation Bruker rapifleX MALDI-TOF/TOF instrumentation we have delivered analysis read times of <0.25 sec/sample with sample volumes as low as 25nL. MALDI targets (with no pre-marked locations) were spotted with a “matrix/analytes/matrix” sandwich in a time frame comparable to rapifleX read time, allowing sample deposition and analysis in less.

Ergebnisse und Diskussion

Using this workflow we have generated a fully automated sample deposition/analysis system with the potential to complete a full diversity 2 million compound primary screen within 8 days. Our data demonstrates highly comparable values when compared to the well established Agilent RapidFire MS technology, but with analysis speeds more suited to HTS and uHTS. Additionally, the direct-detection of MALDI-TOF MS mitigates the need for extensive confirmatory assays commonly needed with fluorescent-based technologies, as well as reducing both cost and assay development time commonly associated with fluorescent technologies (i.e. the development of specific fluorescent probes or antibodies). Furthermore this technology and workflow can be applied across different targets and applications and has the potential to significantly impact on the productivity of early drug discovery and development.

Neue Aspekte

Fully Automated ultra High Throughput Screening
based on MALDI TOF MS allows more than amillion assay spots
to be screened

The performance of mobile GC-MS for field sampling of body odours from common marmosets (Callithrix jacchus)

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The analysis of signals emitted and received by individuals has always been of great interest in behavioural science. Within this context, volatile compounds are of highest relevance to understand olfactory communication within and between species. However, due to their motility, rapid *in situ* sampling is required to analyse the odour of animals. Therefore, state of the art methods trap volatiles on adsorption materials and subsequently analyse these samples by GC-MS in an off-site lab. In contrast, recently developed mobile GC-MS devices with direct probes could enable the analysis of body odours without additional materials. We compare these two methods to find the most suitable method for investigation of olfactory communication in free-ranging animals.

Experimenteller Teil

Body odour samples from six female common marmosets (*Callithrix jacchus*) were collected in parallel

- analysed on a stationary GC-MS (Shimadzu TQ8040 and Leco Pegasus III) after active sampling with an air pump to tubes containing:

- two adsorption materials, Tenax TA® and XAD-2,
- either Tenax TA® or XAD-2

- by direct air sampling onto the device-inherent trap of a mobile GC-MS device, Hapsite ER (Inficon, Cologne, Germany).

The maximum flow rate for each approach (~ 1 L/min for the tubes and 100 mL/min for the Hapsite ER) was used to sample a total volume of 6 L and 300 mL, respectively. Data evaluation was carried out as average comparison of six independent replicates.

Ergebnisse und Diskussion

In the first part of the evaluation, we present the compound coverage obtained with both methods applied to body odour analysis of common marmosets. As expected, the analysis of volatiles collected from the thermodesorption tubes appear to be more sensitive in comparison to the results achieved with the mobile device. We show to what extent the detected compounds match each other and compile the information that would be lost using only either one of the methods.

In a second part, we evaluate the relative composition of the samples to see whether quantitatively different compound profiles are obtained with both methods. For this comparison, we consider only those compounds which were detected with both sample

collection approaches. The differences in these profiles are very likely related to the fact, that the volatiles feature different recovery rates during adsorption to the collection tube materials.

In addition, we present a discussion comparing the handling these two methods of sample collection for field studies and the resources required. According to the putative identification by EI-MS library search, the fraction of compounds potentially originating from or metabolized by the individual, respectively, related to those originating unambiguously from the ambience was between 50 to 70%, an important fact when it comes to a rating of the usefulness of both methods for the purpose of sampling body odour from animals.

In comparison to the mobile GC-MS device, active sampling by an air pump using thermal desorption tubes subsequently analysed with a standard lab GCMS is concluded to still be the most appropriate approach for VOC analysis in field studies.

Neue Aspekte

The performance of a mobile GC-MS for VOC analysis is compared to the standard sampling method by thermal desorption tubes.

Analysis of Glycoproteins with different LC-MS/MS and NMR techniques

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Abstract

Glycosylation of proteins is one of the most important post translational modification (PTM) since glycosylation influences the biological function of proteins. Alterred glycosylation was found in many diseases, eg cancer or inflammatory disease. Hence, anylasis and quantification of glycan structures is very important to get a better understanding of structur related function, for developement of biomarkers or qualtiy control of biopharmaceuticals. Here, we present different approaches to analyse glycosylation and quantify glyosylation patterns of human ceruloplasmin from single individuals. A middle down approach was used to obtain glycosite specific information and quantify PTMs. Further fragmetation with *in source collison induced decay* gave information about amino acid sequnce and glycan linkage. Next to PTM analysis, it was possible to detect different gene variants and quantify the ratio of natural protein variant and variants with amino acid excange.
For a complete identification, *N*-glycans were cleaved by PNGase F and analysed by LC-MS and ^{1}H-NMR, allowing determination of linkage position and anomericity. Chromatographic overlap of compunds was overcome by using the 3DCC (*three dimensional cross correlation*) method invented in our lab to calculate pure nmr spectra from compund mixtures.

Identification of PTMs with middle down proteomics

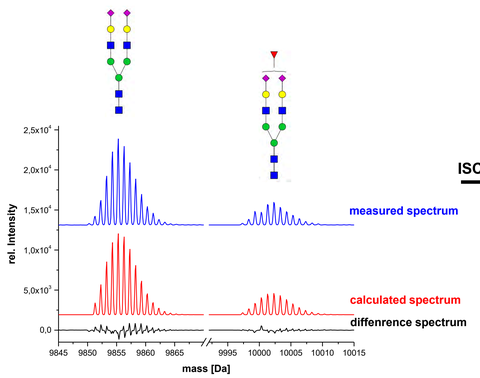


Fig. 1.: Deconvoluted spectrum for protein fragment ^{111}Asn to ^{177}Arg including one glycosite at ^{138}Asn. Measured spectrum is shown in blue, calculated spectrum in red. Two different glycoforms could be identified.

ISCID fragmentation

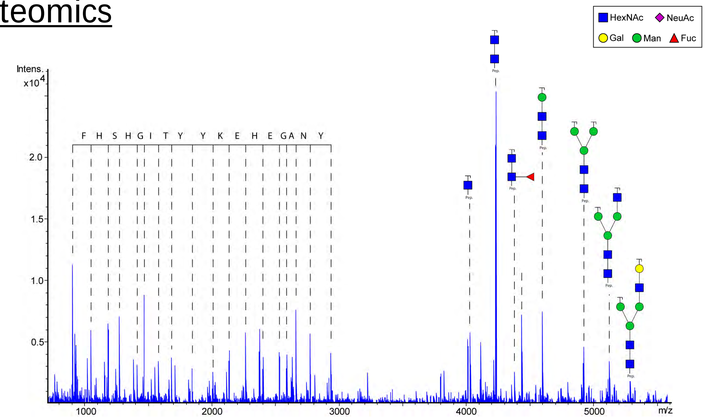


Fig. 2: Fragment spectrum (ISCID) for protein fragment ^{111}Asn to ^{177}Arg. The spectrum not only shows fragmentation of glycan residue but also fragmentation of peptide residue (y-fragments marked with one letter code).

Analysis of glycosylation pattern from human ceruloplasmin was performed with a middle down approach, having the advantage of glycosite specific information compared to a top down analysis. Incomplete tryptic digest led to protein fragments between 10 and 30 kDa respectively. Fig. 1 shows the deconvoluted (maximum entropy) spectrum for the protein fragment from ^{111}Asn to ^{177}Arg including two differrent glycoforms at glycosite ^{138}Asn (blue). Calculation of the spectrum (red) indicate a ratio of 1.7:1.0 for the non fucosylated and the fucosylated specie. Ionisation properties of the two glycopeptides were set as equal due to their huge structural similarity (98.5 %).

The same protein fragment was further fragmented by *in source collision induced decay* (ISCID). The deconvoluted fragment spectrum (Fig. 2) not only showed fragmentation of the glycan residue like normal CID fragmentation experiments with glycopeptides but also fragmentation of the peptide residue. The fucose could be identified as proximal.

Analysis and quantification of SNPs and PTMs

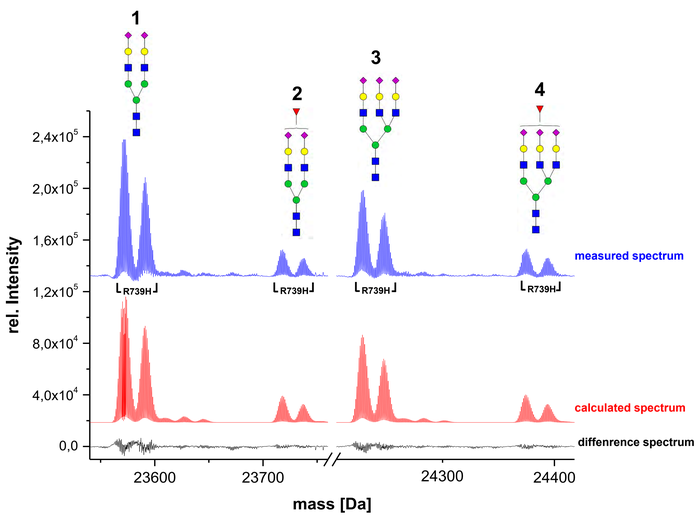


Fig. 3.: Deconvoluted spectrum for protein fragment ^{639}Gly to ^{821}Lys including one glycosite at ^{762}Asn. Measured spectrum is shown in blue, calculated spectrum in red. The spectum shows two signals for each of the four identified glycans (structures 1 to 4) due to an amino acid exchange at R739H. Hence, the donor carries a point mutation heterozygot. Glycosylation is not affected.

As mention aboved, middle down proteomics has several advantages compared to top down or bottom up approaches. Human ceruloplasmin from one individual was analysed with the same method. The sample showed two SNP's (*single nucleotide polymorphism*) heterozygot. One SNP led to the amino acid change R739H (variant rs115552500) wich is assumed to correlate with a higher risk of neugenic diseases like parkinson. Fig. 3 shows the deconvolutet (maximum entropy) sprectrum for the protein fragment ^{639}Gly to ^{821}Lys including four different glycoforms at glycosite ^{762}Asn (blue). Calculation of the spectrum (red) indicate a ratio of 1.5:1 for the variant with the SNP and the natural variant over all 4 glycan signals. This difference in serum protein concentration can be explaind with eg different expression rates or clearence rates for one variant over the other.

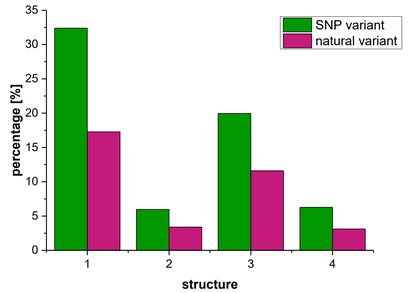


Fig. 4: Quantification results for protein fragment ^{639}Gly to ^{821}Lys . Structures 1 to 4 correspond to glycan structures shwon in Fig. 3. Quantifiction was done by comparing the weightning factors of the calculated spectrum.

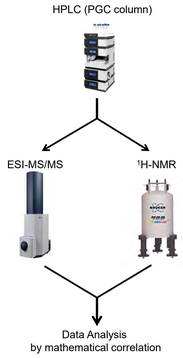
Next to the quantification of protein ratio (natural variant against variant with SNP), the spectrum shows the same glycosylation pattern for both variants, clarifying that the amino acid exchange has no effect on glycosylation. Fig. 4 shows the results of quantification over all 4 glycan signals for the variant with SNP (green) and the natural variant (purple).

Free Glycans - unambiguos assignment with LC-MS and NMR

Structure determination of complex glycans is very challenging due to their varietiy of isomers. Nevertheless linkage position and anomericity play an important role in many biological functions. Here, we present a complete characterisation of released *N*-glycans from human ceruloplasmin from one individual using the combination of LC, MS and NMR data.

The workflow includes the chromatographic separation of glycans on a porous graphitized carbon (PGC) column with online MS/MS analysis on an ESI-q/TOF mass spectrometer. The LC flow is simultaneously splited and fractionated for offline ^{1}H-NMR analysis. Since a perfect chromatographic separation is almost always impossible, we invented a method called **3DCC** (*three dimensional cross correlation*) for calculation pure NMR spectra from overlapping compounds by correlating the extracted ion chromatograms (EIC) (*first dimension*) with the extracted delta chromatograms (EDC) (second dimension) over their shared retention time dimension (*third dimension*). The correlation can be done with a least square optimization or with correlation coefficients (Pearson).

In this example the complex biantennary structure and the triantennary structure show a chromatographical overlap between 26.5 to 30.5 min on a PGC column (Fig. 5). Applying the 3DCC method, it was possible to obtain pure NMR spectra for both compounds and determine linkage position and anomericity.



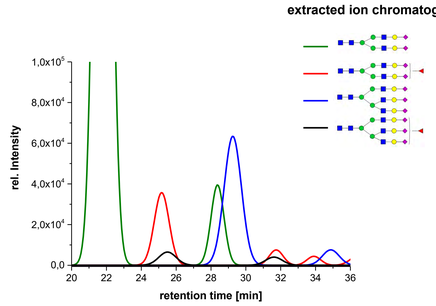


Fig. 5: LC-MS chromatogramm for eluting glycans on a PGC column. EICs between 26.5 and 30.5 show a huge overlap.

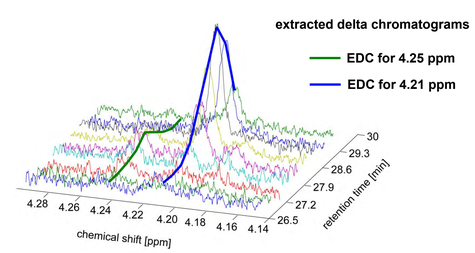


Fig. 6: Excerpt of NMR spectra from fractions between 26.5 and 30.5 min. EDCs for 4.25 ppm and 4.21 ppm show the same chromatographic behaviour as the corresponding EICs.

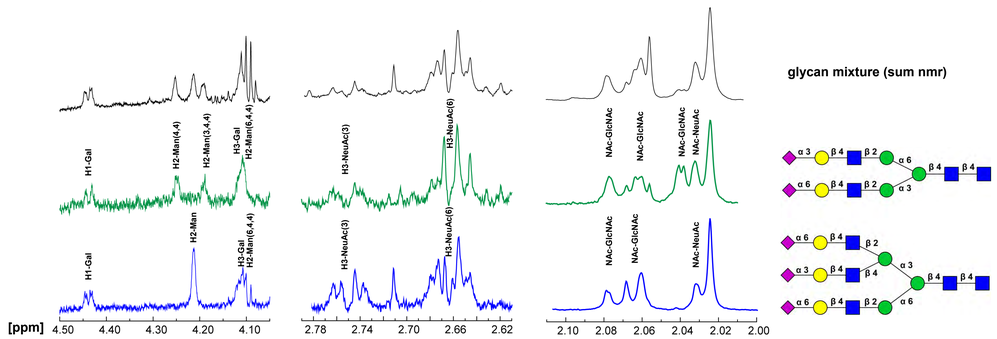


Fig. 7: Exerpt of the calculated NMR spectra for the biantennary (green) and triantennary (blue) glycan. The sum spectra over all compunds is shown in black. After calculation of pure nmr spectra, signals could be assigned to their corresponding glycan structure. Notably, the signals from H2 of the mannoses shift between biantennary and triantennary structure (shown between 4.30 ppm to 4.15 ppm). Calculation of pure NMR spectra via 3DCC is demonstrated for glycans but can be applied to many types of analytes.

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Identification of an unusual *N*-glycan detected in a tryptic glycopeptide derived from intergrin α7 expressed in *Drosophila* S2 cells

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Proteins for scientific or therapeutic purposes (e.g. vaccines) are frequently cloned and expressed in continuous insect cell lines. However, in case of glycoproteins, the structures of *O*- and *N*-glycans are determined by the glycosylation machinery of the expression system. The production of proteins in insect cells mostly generates α1-3 and/or α1-6 fucosylated *N*-glycans of the pauci mannose type. In the course of the present study a hitherto unknown *N*-glycan comprising a phosphoethanolamine (EtnP) and a hexuronic acid residue was identified in a tryptic peptide derived from integrin α7 expressed in a *Drosophila* cell line.

Integrin α7 was expressed in *Drosophila* Schneider 2 (S2) cells and isolated by affinity chromatography. After SDS PAGE the corresponding band was excised and the protein was subjected to an in-gel tryptic digestion. The (glyco)peptides obtained after extraction and purification were analyzed by nanoESI mass spectrometry using a Synapt GS2 instrument.

The majority of the glycans detected in tryptic glycopeptides derived from S2-expressed integrin α7 were pauci mannosidic and a few of them were extended by one GlcNAc residue. A low-energy CID experiment on the 4 times charged precursor ions ($[M+4H]^{4+}$) at *m/z* 1215.52 yielded Y ion series that clearly demonstrated the presence of a core monofucosylated pauci mannosidic structure elongated by a single GlcNAc. However, there was a gap of 461.10 u from the last Y ions to the precursor ions that could not be filled with increment combinations of conventional *N*-glycan monosaccharides (Hex, HexNAc, Fuc, NeuAc, etc.). B ion (*m/z* 286.07, 462.10, and 665.18) and C ion (*m/z* 142.03, 304.08, and 480.11) series evidenced the sequence EtnP-Hex-HexUA-HexNAc. Moreover, EtnP-Hex-HexUA gave rise to an increment of 461.10 u (vide supra) and the presence of EtnP was corroborated by neutral losses of 43.04 u ($NH_2{-}CH{=}CH_2$) from B ions which are typical for EtnP-containing compounds. Merging all data obtained a glycan structure of $GlcNAc_2(Fuc)Man_3GlcNAcHexUAHexEtnP$ was deduced. Three times charged Y_0 ions (peptide) at m/z 1052.83 as well as a few detectable b and y ions demonstrated that the peptide backbone consists of aa695-723 and contained an intramolecular disulfide bridge. Finally the calculated *m/z* 1215.5118 for the entire glycopeptide is in excellent agreement with the experimental value of *m/z* 1215.52.
The present study demonstrates that careful examination of the glycosylation of heterologous expressed proteins may lead to the detection of unexpected glycan structures. This could be crucial with respect to altered physicochemical properties and antigenicities of the expression products caused by host-specific glycosylations.

Key words
N-glycosylation, heterologous expression, nanoESI MS, CID

Novel aspects
A novel *N*-glycan was identified on a tryptic glycopeptide from intergrin α7 expressed in *Drosophila* S2 cells by nanoESI CID.

Mass spectrometric characterization of aberrant O-glycosylation in COSMC deficient mouse pancreas tissue

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A frequent observation in pancreatic cancer is an aberrant O-glycosylation of proteins. The high expression of truncated O-glycans, such as the Tn antigen (GalNAcα1-O-Ser/Thr), is associated with poor survival.[1] A malfunctioning T-synthase, the enzyme responsible for extending O-glycan core 1 structures, or alterations in its essential chaperon COSMC results in an overexpression of Tn antigen. To gain further insight into the relation between aberrant O-glycosylation and pancreatic cancer a conditional COSMC-KO mouse model was generated. In this study, pancreatic tissue from these mice was used to enrich Tn antigen bearing proteins and characterize them by LC-MS/MS.

Experimenteller Teil

Pancreatic tissue from COSMC-KO mice was homogenized and tryptically digested following a filter aided sample preparation protocol (FASP).[2] The peptides were treated with neuraminidase and PNGase F. Tn antigen bearing peptides were subsequently enriched with *Vicia villosa* agglutinin (VVA) using a filter aided protocol. Additionally, enrichment at protein level with VVA conjugated agarose beads was performed, followed by tryptic digestion. Peptide samples were measured on a nanoHPLC coupled to an Orbitrap mass spectrometer. Data was processed using MaxQuant.

Ergebnisse und Diskussion

Upon HCD fragmentation, GalNAc moieties usually dissociates from the peptide before the peptide backbone is fragmented and can form oxonium ions. These oxonium ions can be used as diagnostic ions, giving evidence of modified precursor ions. The data was searched for the presence of the GalNAc oxonium ion signal at m/z = 204.087. Filter aided VVA enrichment at peptide level yielded far more MS/MS spectra containing a diagnostic ion signal at m/z = 204.087 than enrichment at protein level did. MaxQuant identified GalNAc-modified peptides and manual revision of corresponding MS/SM spectra confirmed the findings. For example, the peptide RVET*VQNHQR (precursor = m/z 735.31) from Intraflagellar transport protein 81 could be identified to bear a truncated O-glycosylation. Although we were able to identify some aberrant O-glycosylated proteins the VVA enrichment has to be improved further.

Neue Aspekte

Enrichment and characterization of aberrant O-GalNAc (Tn antigen) modified proteins in COSMC-KO mouse pancreas tissue.

Referenzen

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INCREASED CONFIDENCE FOR THE IDENTIFICATION OF N-LINKED GLYCOPEPTIDES USING AN OPTIMISED COLLISION ENERGY WORKFLOW

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INTRODUCTION

Glycosylation is responsible for the regulation of cell-cell interactions, recognition and diseases. The development of viable glycomarkers has been limited due to the technical challenges raised from sample preparation and analytical methodologies. Mass spectrometry (MS) is seen as an important tool for elucidating glycan structure but can prove challenging from a data acquisition and processing perspective. For example, N-glycosylated peptides often provide intense Y and B fragment ions corresponding to the carbohydrate moiety when fragmented by means of collision induced dissociation (CID). This is counteracted with inefficient fragmentation of the peptide backbone. Therefore having the ability to customise the collision energy (CE) applied to glycopeptides would be advantageous. Here we describe an LC-MS method which provides efficient glycan and peptide backbone fragmentation within a single acquisition using optimised collision energies.

METHODS

Sample preparation

α-fetoprotein (AFP) and HeLa membrane samples were reduced, alkylated, dephosphorylated and digested using trypsin. Resulting peptides were subsequently enriched using HILIC chromatography. The collected eluent was dried and prepared for LC-MS by resuspending with water:acetonitrile (97:3)/0.1% formic acid.

LC-MS setup

Glycopeptides were chromatographically separated over a 60 min gradient from 5 to 40% acetonitrile (0.1% formic acid) at 300 nL/min using an ACQUITY M-class, configured with HSS 1.8 µm C18 reversed phase 75 µm x 20 cm nanoscale LC column.

MS data were acquired using a Synapt G2-*Si* operating in both data dependent (DDA) and data independent (DIA) modes of acquisition (Figure 1).

Bioinformatics

Data were processed using either Mascot Distiller (DDA) or ProteinLynx Global Server (DIA) for peak picking prior to glycopeptide identification using Byonic and MAGIC (Figure 2).

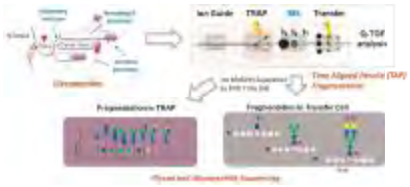


Figure 1. Glycopeptide data acquisition using a Synapt G2-Si Q-IMS QToF mass spectrometer.

RESULTS

Comparison of various CE for N-linked glycopeptides purified from AFP, showed a modest CE of 40eV provided optimal fragmentation from the peptide backbone (b and y ions), whilst a CE of 50eV (trap) yielded rich spectral information for intact glycopeptides. Comparison of transfer based fragmentation, showed that a CE of 50-60 eV yielded good peptide and glycan fragmentation (Figure 3). Confident glycopeptide identifications resulting from Byonic and MAGIC are provided in Figure 4.

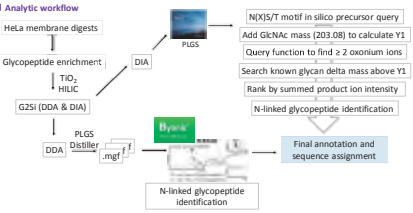


Figure 2. Experimental and data analysis workflow. Data processing uses either PLGS (DIA) or Mascot Distiller (DDA) for peak picking prior. Spectral outputs are further interrogated using Byonic and Magic software for glycopeptide identification and scoring.

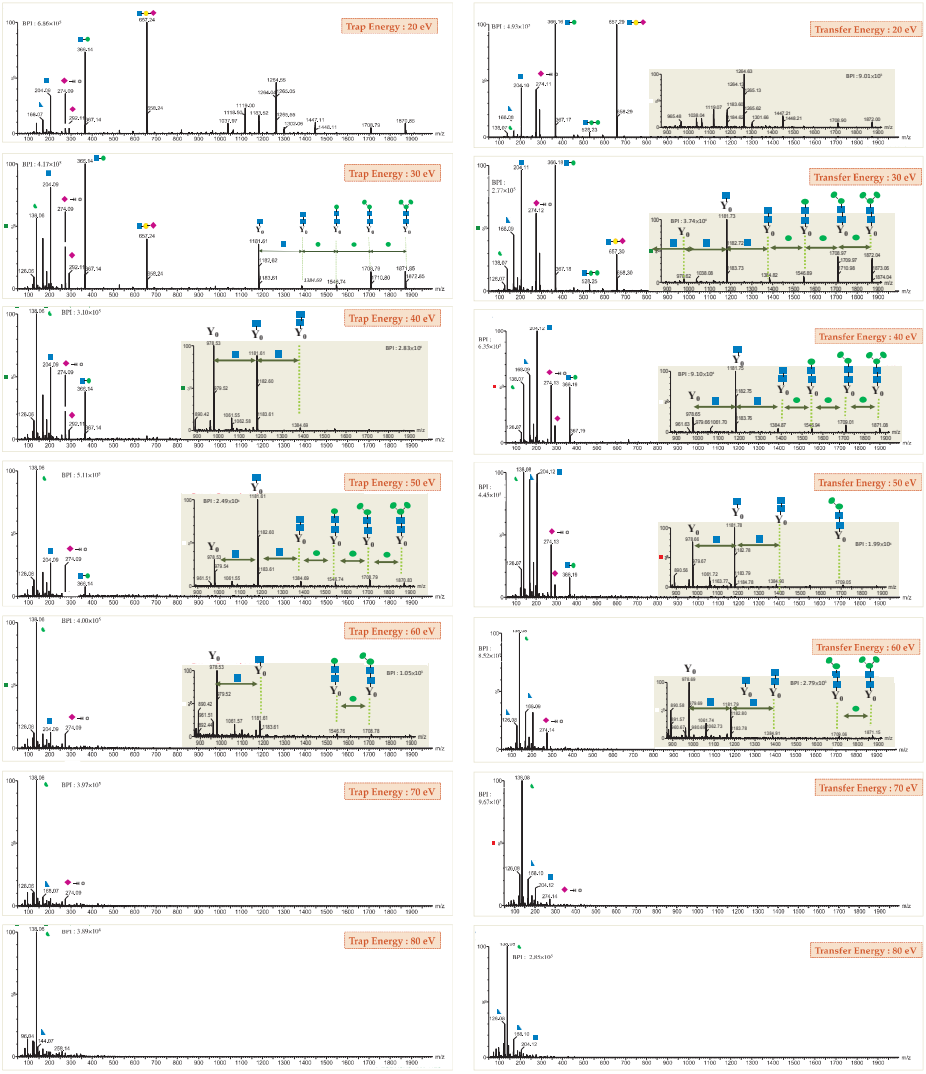
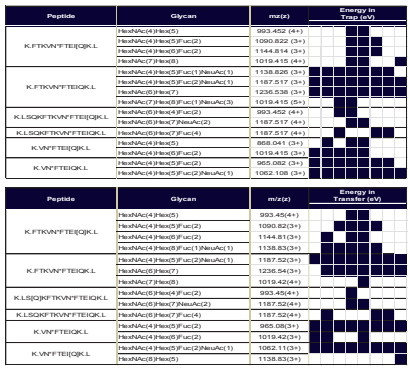
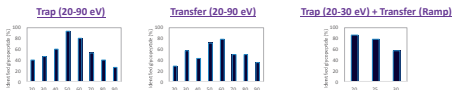


Figure 3. Glycopeptide fragmentation of α-fetoprotein (AFP) at various collision energies (20-80 eV). Comparative fragmentation profiles are shown for the trap and transfer regions of the Synapt G2-Si.



Peptide	Glycan	m/z(z)	Energy in Trap (eV)
K.FTKVNFTEIQIK.L	HexNAc(4)Hex(5)	993.452 (4+)	
	HexNAc(4)Hex(5)Fuc(2)	1090.822 (3+)	
	HexNAc(4)Hex(5)Fuc(2)	1144.814 (3+)	
	HexNAc(7)Hex(8)	1019.415 (4+)	
K.FTKVNFTEIQK.L	HexNAc(4)Hex(5)Fuc(1)NeuAc(1)	1138.826 (3+)	
	HexNAc(4)Hex(5)Fuc(2)NeuAc(1)	1187.517 (3+)	
	HexNAc(6)Hex(7)	1236.538 (3+)	
	HexNAc(7)Hex(8)Fuc(1)NeuAc(3)	1019.415 (5+)	
K.LSQKFTKVNFTEIQIK.L	HexNAc(6)Hex(4)Fuc(2)	993.452 (4+)	
	HexNAc(6)Hex(7)NeuAc(2)	1187.517 (4+)	
K.LSQKFTKVNFTEIQK.L	HexNAc(6)Hex(7)Fuc(4)	1187.517 (4+)	
K.VNFTEIQIK.L	HexNAc(4)Hex(5)	868.041 (3+)	
K.VNFTEIQK.L	HexNAc(4)Hex(5)Fuc(2)	1019.415 (3+)	
	HexNAc(4)Hex(5)Fuc(2)	965.082 (3+)	
	HexNAc(4)Hex(5)Fuc(2)NeuAc(1)	1062.108 (3+)	

Peptide	Glycan	m/z(z)	Energy in Transfer (eV)
K.FTKVNFTEIQIK.L	HexNAc(4)Hex(5)	993.45(4+)	
	HexNAc(4)Hex(5)Fuc(2)	1090.82(3+)	
	HexNAc(4)Hex(5)Fuc(2)	1144.81(3+)	
	HexNAc(4)Hex(5)Fuc(1)NeuAc(1)	1138.83(3+)	
K.FTKVNFTEIQK.L	HexNAc(4)Hex(5)Fuc(2)NeuAc(1)	1187.52(3+)	
	HexNAc(6)Hex(7)	1236.54(3+)	
	HexNAc(7)Hex(8)	1019.42(4+)	
K.LSQKFTKVNFTEIQK.L	HexNAc(6)Hex(4)Fuc(2)	993.45(4+)	
	HexNAc(6)Hex(7)NeuAc(2)	1187.52(4+)	
K.LSQKFTKVNFTEIQK.L	HexNAc(6)Hex(7)Fuc(4)	1187.52(4+)	
K.VNFTEIQK.L	HexNAc(4)Hex(5)Fuc(2)	965.08(3+)	
K.VNFTEIQK.L	HexNAc(4)Hex(5)Fuc(2)NeuAc(1)	1019.42(3+)	
	HexNAc(8)Hex(5)	1138.83(3+)	



protein Entry	peptide sequence	Site	Glycan	mz	z	precursor intensity
ASPH	SSGNSSSSGSGSSTSAGSSSPQAR	11	Hex1HexNAc5NeuAc2+Hex3HexNAc2	951.97	5	2737
CD168	NATGDYK	305	HexNAc1+Hex3HexNAc2	932.87	2	1699
ESYT2	LEWLTLMPNASNLDK	510	HexNAc1NeuAc1+Hex3HexNAc2	963.14	3	1769
G3BP2	GDMEQNDSDNNRR	316	DecoyHex1Hex2HexNAc2+Hex3HexNAc2	806.31	4	780
GNAS1	NCLYGNMISGQR	4	DecoyHex1Hex1HexNAc1+Hex3HexNAc2	945.70	3	1348
GSK3A	VIQNGSFGVVYQAR	126	HexNAc1NeuAc1+Hex3HexNAc2	1275.51	3	1328
IF4A3	EANFTVSSMHGDMPQK	300	Hex1HexNAc1NeuAc1+Hex3HexNAc2	1110.11	3	792
IQGA1	LIFDMPQNKSTK	995	DecoyHex1HexNAc2NeuAc1+Hex3HexNAc2	1058.13	3	4048
ITA1	VQRNITVR	747	HexNAc1+Hex3HexNAc2	1041.00	2	2647
ITA3	NITNTGAPR	264	HexNAc1+Hex3HexNAc2	713.01	3	1229
ITB1	KNKNVTNR	91	HexNAc1+Hex3HexNAc2	690.65	3	10786
ITB1	NGVNGTGENGR	402	Hex1+Hex3HexNAc2	1094.94	2	1138
ITB4	LVNITIK	979	DecoyHex1Hex1HexNAc1+Hex3HexNAc2	580.04	4	1075
ITB4	RLVNITIK	979	Hex1HexNAc1+Hex3HexNAc2	582.79	4	1816
K1C9	GVLDNLTMEK	265	DecoyHex1Hex2HexNAc2+Hex3HexNAc2	1488.13	2	1002
LAMP1	NGNGTACIMANFSAAFSVNYDTK	34	HexNAc1+Hex3HexNAc2	1189.49	3	807
LAMP1	LLNINPNK	256	Hex1+Hex3HexNAc2	990.46	2	3576
LAP2A	MAAHTMGNATVGR	644	DecoyHex1Hex2+Hex3HexNAc2	670.78	4	1284
MAPK2	TTFTPSTNSVLSTSTNRSR	472	DecoyHex1Hex1HexNAc1+Hex3HexNAc2	905.74	3	3727
MRP1	GVNLSGGQK	766	DecoyHex1Hex2NeuAc2+Hex3HexNAc2	935.04	3	520

Figure 4. Identification of AFP glycopeptides. Peptides with associated glycans are tabulated (top/bottom left) indicating the collision energy required in order to observe sufficient diagnostic ions for confident identification. The percentage of identified glycopeptides based on collision energy (top right) show trap and transfer fragmentation to optimize at 50-60 eV. A large percentage of glycopeptides identifications are also shown to result from a combination of trap and transfer collision energies, whereby the transfer ramps 19-45 eV. Example identifications generated for the HeLa membrane digest using the same methodology is also demonstrated (bottom right).

CONCLUSIONS

- **Optimised and sequential CE (i.e. using both trap and transfer) is shown to be important for glycopeptide characterization, ensuring comprehensive profiling of both the peptide backbone and glycan moiety.**
- **A combined DDA and DIA approach has shown to provide good decomposition of glycan structures and peptide sequencing from intact glycopeptides, thereby providing a more comprehensive sequencing.**
- **193 intact glycopeptides corresponding to 112 glycoproteins from HeLa membrane digests were identified, including EGFR, CD63, LAMP1/2 and integrin family proteins.**

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Algorithms for the annotation of isotopes, fragments and adducts, applied to HPLC-HRMS metabolomics data for the discovery of novel compounds

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The separation of complex samples with high performance liquid chromatography (HPLC) and the detection with high-resolution mass spectrometry (HRMS) generates gigabytes of information. This data is often processed utilising automatic algorithms, integrated into workflows. MZmine 2 [1] is a tool specifically designed for metabolomics research and untargeted HPLC-MS analysis, providing methods for, e.g., raw data handling, pre-processing, identification and statistical analysis. Through its modular structure, MZmine 2 is readily extendible by new algorithms. In metabolomics research, the identification of unknown MS signals has repeatedly been described as a bottleneck.[2] To address this issue, two new identification algorithms were developed and integrated in an MZmine 2 workflow.

Experimenteller Teil

A new deisotoping algorithm is applied after an alignment of features (chromatographic peaks with a specific accurate mass-to-charge ratio) throughout a sample set. ^{13}C-isotopologues are grouped based on their accurate masses, by comparing features and searching the raw data for missing signals. Subsequently, features and their intensity profiles in retention time dimension are correlated and grouped by a second algorithm. In this process, putative adducts and in-source fragments are annotated. Both algorithms are fully integrated into an MZmine 2 workflow and were applied to differential metabolomics datasets, acquired in both negative and positive polarity on an LTQ-Orbitrap XL instrument.

Ergebnisse und Diskussion

The advanced new deisotoping algorithm outperformed the standard MZmine 2 method with charge state detection rates of up to 55.4 % compared to 14.5 %, respectively. These results aided a subsequent grouping and correct annotation of features derived from the same molecule. Manual exploration of statistically chosen feature groups was performed in a specifically designed dialogue. The algorithm annotated seven of eleven grouped features with all annotations pointing to the same accurate mass and adduct formation. Similar results were achieved on a dataset acquired in negative polarity with up to five related annotations in a group. The extracted information and visualisation significantly improved the identification process by lowering time consumption and increasing confidence generated by related annotations. Consequently, this lead to the postulation of two novel natural products from *Fusarium fujikuroi*, which are under further investigation.

Neue Aspekte

Two new identification algorithms for MZmine 2 operating with aligned feature lists. A new identification dialogue for manual inspection.

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Themen: MS - Informatik / Bioinformatik, Metaboliten & Metabolomics
Stichworte: HPLC, high-resolution mass spectrometry, Metabolomics, MZmine 2, Algorithm

Simulated microgravity triggers transient enhancement of protein glycation and oxidation in germinating *Brassica napus* seeds

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Introduction

Simulated microgravity is widely used to address the physiological effects of alternating gravity vector, i.e. the factor, expected to accompany humans during inhabitation of space. This experimental setup is helpful in understanding the fundamental mechanisms of polar plant growth and development. Most often, it is applied by a continuous rotation of a plant around one or a several axes using clinostats or random positioning machines. Obviously, clinorotation can be considered as an environmental stress. In this context, enhanced rates of protein glycation and oxidation can be expected [1]. Here we report, to the best of our knowledge, for first time the changes in *B. napus* glycated and oxidized proteome during seed germination under the conditions of simulated microgravity.

Experimental section

The germinating seeds of *B. napus* were subjected to 3D clinorotation in parallel to the corresponding controls grown under the constant growth vector. The seedlings were harvested in liquid nitrogen at 24 and 48 h after germination and grounded with a ball mill. Quantification of stress markers and antioxidants relied on a panel of established spectrophotometric assays. The changes in proteome were addressed by LC-based bottom-up approach employing high-resolution nanoLC-ESI-MS data-dependent acquisition (DDA) experiments. Peptide identification and protein annotation relied on the search against an *A. thaliana* database with manual verification. To characterize microgravity-induced changes in protein functional state and in patterns of prospective protein modification agents (sugars and related compounds) primary metabolome analysis was performed by GC- MS.

Results and discussion

In general, our experiments revealed no effect of clinorotation on seed germination rates. After a 24-h treatment, germinating seeds demonstrated no visible alterations in comparison to corresponding controls. Although no morphological changes were observed during the first day of the experiment, the microgravity-related effects could be clearly seen one day later. Thus, the roots of clinorotated seedlings were longer and thicker in comparison to the corresponding controls, and had no constant growth vector. However, a 1.5-2.5-fold up-regulation of stress markers and 16 metabolites (4 sugars, 2 sugar alcohols, 7 amino and 3 carboxylic acids) was observed on the first, but not the second day of the experiment. In contrast, only lysine demonstrated increased abundance on the second experiment day. Proteomic analysis revealed essential microgravity-related quantitative changes in seedling proteome during the whole experiment. The protein modification patterns were monitored for ten glycative and nine oxidative adducts, found earlier in *B. napus* and *A. thaliana* plants [1]. Thereby, N^{ε}-(carboxymethyl)lysine (CML) and methylglyoxal-derived hydroimidazolone (MG-H) were the most abundant AGEs in the seedling proteome. Interestingly, the numbers of glycated and oxidized proteins were increased only on the first day of microgravity treatment, and did not differ from the control values afterwards. It corresponded well to the metabolome data, and indicated a transient character of the oxidative and carbonyl stress accompanying plant response to clinorotation. This finding raises the question about possible regulatory role of observed glycative and oxidative modifications.

Novel aspects

A short-term transient enhancement of protein glycation and oxidation rates accompanies response of germinating *Brassica napus* seeds to simulated microgravity.

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Key words: AGEs, GC-MS, glycation, metabolomics, microgravity, oxidative stress, seed germination, tandem mass spectrometry.

Comparative analysis of the effects of sulfated hyaluronic acid and dexamethasone on the osteoblast differentiation by nanoLC-MS and random forest modeling

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[2]Technical University Dresden, Faculty of Medicine Carl Gustav Carus, Dresden, Germany
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Introduction

The western civilization is facing an aging population and therefore an increase of age-related comorbidities, e.g. diabetes mellitus and osteoporosis. These diseases affect either the bone mineral density or the bone healing capacities, necessitating the application of bone implants after bone fractures in many cases. However, most bone implants in clinical application serve only as stabilizers. Thus, biomaterials that functionally support the bone healing at the molecular level are of highest demand. Glycosaminoglycans (GAG), one of the main components of the extracellular matrix (ECM), are known to be involved in many cellular functions, e.g. adhesion, migration as well as the stem cell fate. Therefore, GAGs are promising candidates for implant coatings to foster the bone healing [1-3].

Methodology

Sulfated hyaluronic acid (sHA1) was shown to enhance the osteoblast differentiation even in absence of dexamethasone (Dex) [4], which is an established substance used in *in vitro* differentiation. To analyze and compare the molecular effects of both treatments, human bone marrow stromal cells (hBMSC) were labeled by SILAC and differentiated in presence of sHA1 or Dex. Furthermore, to assess potential additive effects of both substances, a double treatment was conducted. The protein composition of the osteoblast-released matrix vesicles (MV) and the cellular proteome were analyzed by LC-MS/MS as described elsewhere [3]. To extract and identify decisive protein groups, correlated to a single or combined treatment from a high density dataset, a random forest modeling (RFM) with subsequent clustering was conducted.

Results and discussion

Both a treatment with sHA1 or Dex induces the osteoblast differentiation represented by an induced activity of the tissue non-specific alkaline phosphatase (TNAP) and subsequent ECM mineralization. Additionally, a combined treatment further enhances this differentiation.
The osteoblast-released MVs were shown to hold a key role in the ECM mineralization [3]. All treatments affect the MV protein composition dramatically, while having only minor effects on the cellular proteome. However, the effects of the Dex treatment highly dominate over effects induced by sHA1 – especially in the combined treatment – hampering the statistical proof and separation of unique effects from additive/synergistic effects. Furthermore, an analysis on single protein level was insufficient to comprehensively reveal the molecular effects of the treatments. By applying RFM, a subset of 113 decisive proteins capable of separating the sample sets gained from single treatments and the combined treatment, could be obtained (OOB error < 0.05). Finally, an integrative analysis of protein clustering based on the treatment response and a classical proteomic analysis lead to a grouping of proteins being (i) mainly affected by sHA1 (N=73) or Dex (N=164), (ii) consistently affected by sHA1 and Dex (N=15) or (iii) showing and additive (N=61) or synergistic (N=41) response. Downstream functional analyses revealed that both sHA1 and Dex treatment induces the cell/ECM interaction. However, while sHA1 mainly affects extracellular proteins and ECM binding proteins, Dex induces the intracellular linkage of receptor proteins to the cytoskeleton. Furthermore, Dex induces many metabolic pathways. Proteins being affected in an additive or synergistic manner show an enrichment in binding to carbohydrates/GAGs and growth factors, e.g. TGF-beta. This may suggests a modulation of proteins being involved in scavenging and/or presenting growth factors by the ECM.

New Aspects

This study provides the first comparative analysis of the established Dex-induced hBMSC differentiation to an alternative approach.

Keywords

Bone healing, proteomics, SILAC, random forest modelling, bioinformatics

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Age-related formation of advanced glycation end products (AGEs) in root nodules of common beans (*Phaseolus vulgaris)*

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Introduction (120)

Glycation is referred to as interaction of protein lysyl and arginyl residues with carbonyl compounds. In the later steps of this process, advanced glycation end products (AGEs) are formed [1]. These modifications underlie aging in mammals, by direct modulation of cellular structure and functions [2]. Recently, formation of AGEs was demonstrated also in plant proteins [3]. This fact raises the question, if ageing is accompanied by glycation in plants as well, and if this process affects plant physiology. Plant-microbial interaction, like symbiosis between legume plants and rhizobia, taking place in specialized organs – nodules, might be one of such physiological aspects. Here we address the dynamics of AGE accumulation during ageing of *Phaseolus vulgaris* nodules and characterize accompanying changes in proteome.

Experimental (120)

AGE-modified proteome of common bean (*Phaseolus vulgaris)* root nodules was characterized by the LC-based bottom-up proteomic approach. To address the age-related changes in the advanced glycation patterns, young, flowering and senile plants were analyzed. For this, the total protein fraction was isolated from the frozen nodule material by phenol extraction, digested by trypsin and resulting proteins were analyzed by nanoUPLC-Orbitrap-LIT-MS operating in a data-dependent acquisition (DDA) mode. The MS/MS data were analyzed by database search using SEQUEST engine, and sequence identity was confirmed by manual interpretation of the spectra. And the last stage of our research, label-free relative quantification could be applied, to characterize the age-related changes in *P. vulgaris* root proteome.

Results and discussion (300)

It is logic to expect, that aging would result not only in the changes of nodule morphology, but also in the functional status of nitrogen fixing apparatus. Proteomic analysis might give insight in these changes of nodules as the screening of the unique AGE-modified sites, which can be identified by tandem mass spectrometry (MS/MS). Certainly, in the first line, we applied a *P. vulgaris* database. However, the manual verification of confident hits revealed a high level of false positive results. This could be explained by a high representation of bacterial proteome in nodules, incompleteness of the database (i.e. low number of entries), and by the fact, that genomic data was used for the building of the database [4]. Therefore, the search against the *Medicago truncatula* database was performed. We propose that, despite a phylogenetic difference, the degree of the protein sequence homology between the two species is high enough to provide reliable protein identifications. As the genome of *M. truncatula* is sequenced since relatively long time for the legume, the correspondent databases are representative. Thereby, all ten classes of AGEs, that were analyzed here, demonstrated an age-dependent increase in numbers of modification sites. These patterns dominated by CML at all time points. That might clearly indicate accumulation of AGEs in root nodules with plant development. This increase can be explained by the accumulation of sugars in the tissues with plant age [5]. Autoxidation of the sugars may result in formation of reactive dicarbonyls that readily modify protein lysyl and arginyl residues. In parallel, enhanced production of reactive oxygen species (ROS) can be observed. To consider the impact of root sugars in nodule glycation, carbohydrate profiling is being done.

Novel aspect (20)

Accumulation of AGEs was observed in the root nodules of common beans during their life span.

Keywords

AGEs, aging, glycation, mass spectrometry, nodule, *Phaseolus vulgaris*, plant-microbial interaction, proteomics

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Determination of Molecular Formulas from Complex Isotope Pattern

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With the accesibility of modern mass spectrometers the determination of molecular formulas from high resolution mass spectral data has become a routine process in structure elucidation of small molecules.

The calculation of the elemental composition is typically based on the accurate mass of the ^{12}C-Peak. Depending on the mass resolution and the software package used the corresponding isotope pattern are used as an additional criterion for the relevance of a calculated molecular formula.

In this paper the meaning of the mass defects of complex isotope pattern on the calculation of elemental compositions will be discussed as well as the use of ultra high resolved isotopic fine structures.

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Experimenteller Teil

To test the benefit of mass defects for the determination of molecular formulas the following experiments were done:

- comparison of experimental and theoretical data obtained at several mass resolutions (20.000-40.000 and 100.000-250.000)

- determination of the precision of mass defects

- evaluation of the impact of mass defects on the elemental composition calculated by different software packages.

Ergebnisse und Diskussion

Spectra were aquired on different type of instruments (Q-TOF, Orbitrap, FT-ICR) and data evaluation was performed with different software packages. Compounds with a complex isotope pattern such as metalorganic compounds, oligomers and S,N,O, halogen-containing compounds are presented.

The meaning of mass defects on the calculation of elemental formulas depending on the resolving power of the instrument is discussed. Comments on the routine use of ultra high resolved isotopic fine structures are given.

Neue Aspekte

Isotope pattern analysis, mass defect, complex isotope pattern

Optimization of crosslinked peptide analysis on an Orbitrap Fusion Lumos mass spectrometer

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Chemical crosslinking in combination with mass spectrometry is a powerful method to determine protein-protein interactions. This method has been applied to recombinant and native protein complexes, and more recently, to whole cell lysates or intact unicellular organisms in efforts to identify protein-protein interactions on a global scale. In this study, we evaluated traditional non-cleavable and MS-cleavable crosslinkers for crosslinked peptide analysis using an Orbitrap Fusion Lumos mass spectrometer. For MS-cleavable crosslinkers, we also compared different types of fragmentation (CID, ETD) and levels of tandem mass spectrometry (MS2 vs MS3). Our data provided insight to the relative performance of different
crosslinking compounds and acquisition parameters relevant for improving identification of protein-protein interaction sites.

Experimenteller Teil

Different amine-reactive, homobifuctional crosslinkers including disuccinimidyl suberate (DSS), bis-sulfosuccinimidyl suberate (BS3), disuccinimidyl sulfoxide (DSSO) [1] and
disuccinimidyl dibutyric urea (i.e. NHS-BuUrBu-NHS) [2] were compared for protein crosslinking labeling efficiency and crosslinked peptide identification using MS2 and MS3 fragmentation methods. A Thermo Scientific™ Orbitrap™ Fusion Lumos™ mass spectrometer was used for crosslinked peptides analysis. Data analysis was performed by Thermo Scientific™ Proteome Discoverer™ using a XlinkX [3] software node.

Ergebnisse und Diskussion

For both DSSO and BuUrBu, we identified over 40 BSA inter-crosslinked peptides using MS2-MS3 approach compared to less than 20 using MS2 CID for DSSO. We also compared these crosslinkers using an E. coli whole cell lysate. Our results show an increase number of identified peptides after crosslinking using the MS2-MS3 in combination with EThcD
method compared to CID/EThcD MS2 method.

Neue Aspekte

Improve identification of intra- and inter-protein interactions though analysis of chemically crosslinked peptides.

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IMS-DIA-MS Characterisation and IMS-MRM QconCAT Quantitation of the Lipidome and Apolipoprotein Complements of Obesity and Diabetes Cohorts

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Obesity is one risk factor causing excess body fat to be accumulated to the extent that it adversely affects health and life expectancy. Obesity is known to initiate inflammation, which in turn can lead to type 2 diabetes. The exact mechanism as to how this occurs is however not well understood. Here, we describe a lipidomic approach to reveal molecular factors that may be involved in these biomolecular processes. The results of these experiments were complemented with absolute quantitation of the plasma Apolipoprotein complement using QconCAT concatenated signature peptides to identify multi-factorial disease associated components and pathways.

Experimenteller Teil

Plasma samples from three biological states of varying phenotype (control, diabetic and obese) were used with each group consisting plasma from six individuals. Extracts were LC separated and lipidomics data acquired using ion mobility assisted data independent acquisitions. Simultaneously, experimentally derived CCS values using travelling-wave ion mobility were determined. The same samples were also tryptic digested and targeted proteomics data acquired and quantified with the same MS platform using combined ion mobility/mass selected oa-ToF MRM analysis.

Ergebnisse und Diskussion

Ion mobility-derived CCS measurements allowed for improved specificity with the inclusion of drift time, providing additional confidence in the identifications returned.

Normalized label-free quantitation results highlighted differential expression of specific lipid classes. Apolipoproteins are key constituents of LDL and HDL and related to obesity, diabetes, and cardio vascular diseases. The inclusion of IMS in the targeted oaToF MRM workflow increased quantitative precision and accuracy with the results in agreement with expected changes in relation with disease and/or phenotype.

Neue Aspekte

Combined discovery IMS-DIA-MS lipidomics and targeted IMS-MRM proteomics workflow.

Derivatization of low-volatile compounds in aqueous solution and analysis by HS-GC-IMS

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Stichworte: derivatization, headspace gas chromatography, ion-mobility spectrometry, metabolomic fingerprinting

Einleitung

Headspace gas chromatography (HS-GC) allows the analysis of organic compounds directly from aqueous samples. However, the scope of analytes is limited to highly volatile compounds. For an application in metabolomic fingerprinting[1] it is desirable to detect also low-volatile biomolecules such as fatty acids, amino acids or biogenic amines. It was therefore our goal to increase the volatility of these compounds by derivatization to make them amenable to HS analysis. The reagent of choice for the derivatization is methylchloroformate (MCF)[2] since it derivatizes amines, amino acids, carboxylic acids as well as phenols and is compatible with aqueous media. The hyphenation of gas chromatography with ion-mobility spectrometry (GC-IMS)[3] provides 2D orthogonal data with a superior resolution compared to 1D chromatographic separations.

Experimenteller Teil

The analytes (amino acids, amines, fatty acids, phenols) in aqueous solution were derivatized with MCF and subsequently neutralized with 6 M HCl when pyridine was used. HS analyses of the resulting solutions were conducted using an Agilent 6890N gas chromatograph (Agilent Technologies Deutschland GmbH & Co. KG, Waldbronn, Germany) coupled with an IMS-module (G.A.S. Gesellschaft für analytische Sensorsysteme mbH, Dortmund, Germany) and equipped with a MPS2 Multi Purpose Autosampler (Gerstel GmbH, Mühlheim/Ruhr, Germany). The success of the derivatization was also verified by GC-MS analysis (liquid injection). For this purpose, the solution was extracted with diethyl ether after derivatization and the extract was analyzed using an HP 6890 GC/5973 MSD system.

Ergebnisse und Diskussion

All examined compounds were successfully derivatized with MCF as proven by GC-MS analysis. The derivatives of several amines and fatty acids up to myristic acid were detectable by HS-GC-IMS, which was not possible for most of the underivatized analytes. LOD/LOQ were determined in the low to medium µg/L range (*n*-dibutylamine - LOD: 2 µg/L, LOQ: 15 µg/L; hexanoic acid: LOD: 3 µg/L, LOQ: 46 µg/L; octanoic acid: LOD: 23 µg/L, LOQ: 95 µg/L; 4-chlorophenol – LOD: 52 µg/L, LOQ: 296 µg/L). However, derivatives of amino acids and biogenic amines, such as phenethylamine or dopamine were still not volatile enough to be detected by HS-GC-IMS. Future experiments will focus on further biogenic compounds or metabolites and the applicability on metabolomic fingerprinting of fungi.

Neue Aspekte

A new method for the analysis of low-volatile compounds in aqueous solution by HS-GC-IMS is described.

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Analyzing macromolecular complexes: subunit interactions of the F_1F_0 ATP synthase and conformational changes of the heterodimeric ABC transport complex TmrAB

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Introduction:

Life needs energy which cells need to convert from external sources as light or nutrients into adenosine triphosphate (ATP) by a variety of biochemical processes. ATP is a universal energy source of living cells and is used for numerous energy-consuming reactions (e.g. biosynthesis, transport through membranes, regulatory networks and nerve conduction). The major focus for this project is on the ATP depended complex F_1F_0 ATP synthase of *Acetobacterium woodii* and the heterodimeric ABC transport complex TmrAB from *Thermus thermophilus*. Those complexes are characterized by non-covantly bound subunit interactions and could be determined with mass spectrometric methods, especially laser liquid ion desorption (LILBID) or nano-electrospray ionization (nESI).

Experiments:

LILBID-MS is a very soft ionization method, therefore non-covalently bound complexes can be analyzed. Subunit dissociation can be induced in dependence of the desorption laser power. A droplet generator generates droplets of the aqueous sample of a diameter of 30-50 µm at a frequency of 10 Hz. The droplets are transferred into vacuum and irradiated with a mid IR laser pulse which leads to an explosive expansion of the droplets, ionization of the solvated analyte and finally a detection by a time-of-flight (ToF) analyzer[1].

The Synapt G2-S*i* HDMS offers mass spectrometry (MS), tandem-MS and ion mobility (IM) setups. IM measurements in the Triwave region enable the separation of ions of the same mass according to their size, shape and charge.

Results:

In collaboration with the group of Prof. Volker Müller we are focusing on assembly studies of *A. woodii* F_1F_0-ATP synthase and analyzing subunit interactions with LILBID-MS.

Expression, purification and characterization of the wildtype F_1F_0 ATP synthase of *Acetobacterium woodii*

The template plasmid pKB3-His (12453 base pairs) which includes the *atp*-operon of F_1F_0 ATP synthase of *Acetobacterium woodii* was transformed in the ATP synthase negative *E. coli* strain DK8 cells[2]. The purification of the complex was performed with Ni^{2+}-NTA- affinity chromatography. For further analyzation a 12.5 % polyacrylamide gel was prepared and the proteins were visualized by coomassie and silver staining. F_1F_0 ATP synthase complex was then purified by size exclusion chromatography (Superdex 75 100/300 GL).

LILBID-MS at low and high laser energy

At low laser energy the whole F_1F_0 ATP synthase complex could be detected. The increase of the laser energy was coupled to an increase of signal intensity and also dissociation into subcomplexes and subunits. All eight subunits could be observed at high laser energy[3].

First assembly studies of separately expressed subcomplexes are on the way.

Conformational changes of the heterodimeric ABC transporter TmrAB from *Thermus thermophilus* induced by substrate addition

In collaboration with the group of Prof. Robert Tampé we monitored conformational changes of the heterodimeric ABC transport complex TmrAB (4.5 µM) related to substance transport over the transmembrane. Therefore we use ATP/ADP (500 µM) at permissive conditions[4] (incubation: 68 °C, 500 µM MgCl, 5 min).

We analyzed conformational changes in dependence of the bioactivity of TmrAB by different experiments, e.g. vanadate induced trapping[5] and a crosslink mutation.

New aspects:

Subunit interactions in macromolecular complexes. Dependence of the conformational structure of membrane proteins by a variety of substrates.

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Key words:

LILBID-MS, nESI, ion mobility, ATPase, ABC Transporter

The Amyloid Formation Mechanism of Human IAPP: An Infrared Spectroscopy Approach

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The human islet amyloid polypeptide (hIAPP) is a highly amyloidogenic 37-residue peptide hormone produced by the β-cells of the pancreas. Its early oligomerization was shown to be responsible for β-cell death and is increasingly considered as a primary pathological process linked to type II diabetes. In healthy individuals, hIAPP is co-secreted with insulin and stored at a concentration of 1-4 mM, which is 1000-times higher than it is required to form amyloid fibrils in vitro. Thus, insulin might act as an inhibitor for the hIAPP fibril formation in vivo. However, the mode of inhibition as well as the hIAPP assembly pathway is not completely understood and different models are under debate.

Experimenteller Teil

Amyloidogenic oligomers are challenging to characterize using established condensed-phase techniques because they are both polydisperse and polymorph. That is, instead of adopting a defined oligomeric state they form a dynamic equilibrium of multiple species, which also coexist in different conformations. In the present work we used a combination of ion mobility-mass spectrometry (IM-MS) and gas phase infrared (IR) spectroscopy to disentangle the hIAPP assembly pathway and to obtain direct structural information of individual oligomeric species. Absolute collision cross-sections (CCSs) as well as ion mobility- and *m/z*-selected IR spectra of the amyloidogenic human IAPP and the non-toxic rat IAPP counterpart were obtained using an in-house constructed drift tube IM-MS instrument.

Ergebnisse und Diskussion

Recently, the hIAPP and rIAPP peptides were investigated using ion mobility-mass spectrometry and replica-exchange molecular dynamics.[1] The data reveal that the hIAPP monomer adopts two conformations, a compact and an extended one. However, the extended structure is not observed for the non-toxic rIAPP counterpart, leading to the conclusion that this conformer represents an amyloidogenic precursor. Furthermore, the hIAPP dimer is larger in size than the rIAPP dimer and is thus likely formed by the extended hIAPP hairpin conformer. Based on theoretical calculations a helix-coil structure for the compact form and an extended β-hairpin for the extended structure was proposed. In contrast to this, condensed-phased data obtained by CD, NMR or FT-IR spectroscopy instead suggest a transition into amyloids via the formation of helix-rich oligomers.[2]

While IM-MS can investigate individual species, it does not provide direct information about the underlying secondary structure. Conversely, condensed-phase methods are only capable to provide ensemble-averaged information. We used therefore a combination of IM-MS and IR spectroscopy to obtain a detailed structural information of individual conformations and oligomers.

The IR spectra of compact hIAPP and rIAPP monomers show an amide I feature at around ~ 1670 cm^{-1}. In contrast to this observation, the amide I band of the extended hIAPP monomer is observed at ~ 1657 cm^{-1}, which further supports a distinct structure different from the compact version. In addition, the hIAPP dimer amide I band is also observed at ~ 1657 cm^{-1}.

This is in line with the assumption that the dimer formation is initiated by the extended hIAPP monomer structure. Taken together, the data further supports previously reported IM-MS data.

Neue Aspekte

IM-MS combined with IR spectroscopy confirm that the extended hIAPP monomer adopts a different structure than its compact verison.

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Quality assessment of olive oil based on volatile compound fingerprinting using HRGC-IMS analysis

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Stichworte: Authenticity assessment, Fingerprinting, Multivariate data analysis

Einleitung

The evaluation of extra virgin olive oil (EVOO) with respect to quality and authenticity has been in the focus of a plethora of studies in the past years and still poses a challenge for researches. In particular, sensitive, rapid and low-cost analytical methods are highly relevant for enforcement purposes to ensure EVOO authenticity. Non-targeted headspace analysis of volatile organic compounds (VOCs) by high resolution gas chromatography (HRGC), coupled to ion mobility spectrometry (IMS) provides a fast and effective approach for the discrimination of EVOOs of different geographical origins or of different quality categories. This is especially due to minimal sample preparation and short run times, paired with the orthogonal separation power of retention time vs. drift time in GC-IMS.

Experimenteller Teil

All analyses were carried out on a prototype headspace high resolution GC-IMS system with a G.A.S. IMS detector. A defined amount of the olive oil sample was spiked with internal standards and then subjected to headspace analysis. The chromatographic separation was carried out on a mid-polar GC column, using nitrogen as a carrier gas. To interface the GC and the IMS, a heated transfer line was kept at 120°C. The drift tube was operated at constant voltage of 246 V cm^{-1} and a temperature of 90°C under flow of nitrogen at 150 mL/min. Resulting orthogonal data (retention time x drift time) were evaluated with the LAV software by G.A.S. (Dortmund) and with custom MATLAB routines.

Ergebnisse

Headspace high resolution capillary gas chromatography (HS-HRGC) coupled to IMS is a very promising method for the generation of volatile composition profiles for the discrimination of extra virgin olive oils (EVOOs) of different geographical origins. Specifically developed chemometric MATLAB® routines were evaluated. A combination of unsupervised principal component analysis (PCA) with two supervised procedures, linear discriminant analysis (LDA) and k-nearest neighbors (kNN) were applied to experimental data. The results demonstrate, that the information from the high-resolution 3D fingerprints of volatile organic compound (VOC) fractions of EVOO samples is suitable to differentiate between the different olive oil provenances or quality categories in combination with chemometric data assessment. The generated data allowed a non-targeted separation of EVOO samples with the same origin, but different qualities, as well as a tentative separation based on geographical origin. In combination with novel multivariate data analysis techniques, the data generated proved to be superior to the currently used IMS hyphenation techniques. Together with a simplified sample preparation and fast analysis times, HS-HRGC-IMS delivers a cost-efficient experimental setup.

Neuer Aspekte

Application of a prototype HS-HRGC-IMS system for the differentiation of EVOO qualities and origins using non-target fingerprints and multivariate data analysis.

Historical charcoal additions potentially improve stability of soil organic carbon

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Abstract

1. Objective

Improving the stability of soil organic carbon (SOC) and soil's capacity to store SOC are promising ways to mitigate climate change. Recently, several studies showed that additions of charred biomass (e.g. charcoal) elevated SOC stocks and stabilized natural organic matter; however, the mechanisms for C stabilization are hardly known.

2. Material and Methods

We investigated SOC, dissolved organic matter (DOM) and particulate organic matter (POM) of two different soils and their counterparts with former inputs (several decades ago) of charcoal by means of elemental analysis. Further, hot water extracts (HWE) of soils and applied charcoal were investigated by the ESI-FTICR-MS for molecular level details of thousands of inherent organic compounds, solid state NMR is made for soils and charcoal, respectively.

3. Results and Discussion

Charcoal additions increased substantially concentrations of black C, total C and total N in bulk soil, however, concentration of water extractable SOC and N remained unchanged.

Pattern of the POM size fractions changed with a relative increase in the free POM fraction and a decrease in the occluded POM fraction and soil particles <20 µm. However, all POM fractions in charcoal enriched soils were augmented with C and N.

Organic compounds found in HWEs of soils and charcoal contained a broad range of molecules, which highly varied in their polarity and aromaticity. Highly condensed hydrocarbons were found however exclusive in charcoal HWEs. This is in contrast to molecular composition measured of Cambisols and Luvisols, which were generally less aromatic (lignin range only). Surprisingly, differences between molecular composition of soil and their charcoal enriched forms were negligible – in contrast to solid state NMR investigations.

This study confirmed previous findings that charcoal additions increase SOC long-lastingly. Further, an assumed abrasion resistance of charcoal particles may explain elevated free POM fractions, which thereby may act as sorbent of soil organic matter. So stabilized, partially and slowly charcoal ageing under oxidation and hydratisation lead to structures similar to humic acids. A comparison to wildfire influenced soil samples complete the investigations.

New aspects: Charcoal addition with long range depot effect lead to an effective carbon-sequestration in contrast to wild fire clearing.

Key words: ageing, charcoal, extract, FTICRMS, soil

Evaluierung basischer Polypropylenglycole als Standards zur internen Kalibrierung für exakte Massen in der positiv-Ionen MALDI-TOF-MS

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Die matrix-unterstützte Laserdesorption/Ionisation (MALDI) [1] ist besonders verbreitet in der Kombination mit Flugzeitmassenspektrometern (TOF) im Einsatz. Basische Polypropylenglykole (PPGs) einer Gruppe mit der Handelsbezeichnung Jeffamine (Huntsman (Germany) GmbH) wurden bezüglich ihrer Eignung zur Verwendung zur internen Massenkalibrierung für die MALDI-TOF-MS untersucht. Für Direct Analysis in Real Time (DART) wurden eines davon bereits erfolgreich eingesetzt [2,3]. Im Unterschied zu den sonst häufig verwendeten Polyethylenglykolen (PEGs) sind für Jeffamine aufgrund ihrer basischen Amino-Endgruppe bessere Ausbeuten an $[M+H]^+$-Ionen zu erwarten. Mit dem Ziel der Bestimmung exakter Massen in der MALDI-TOF-MS wurden daher vier Jeffamine (M-600, M-2005, D-400, D-230) untersucht. Dieser Beitrag stellt Jeffamine M-2005 als neue Kalibriersubstanz für MALDI-TOF-MS im Bereich *m/z* 200–1300 vor.

Experimenteller Teil

Alle MALDI-TOF-Spektren wurden an einem Bruker Autoflex Speed LRF im positiv-Ionen-Reflektor-Modus, gemessen. Das Gerät wurde mit Bruker FlexControl 3.4 gesteuert und die Spektren mit Bruker FlexAnalysis 3.4 ausgewertet. Die vier Jeffamine (M-600, M-2005, D-400, D-230) wurden von Huntsman (Germany) GmbH zur Verfügung gestellt. Lösungen der Jeffamine von 1 mg ml^{-1} in Methanol wurden mit a-Cyano-4-hydroxyzimtsäure (CHCA), 2,5-Dihydroxybenzoesäure (DHB) oder 2-[(2E)-3-(4-tert-butylphenyl)-2-methylprop-2-enyliden] malononitril (DCTB), jeweils 10 mg ml^{-1}, auf Probenträgern aus Edelstahl präpariert. Das Verhältnis von Analyt- zu Matrix-Lösung variierte von 1:5 bis 1:40. Zur Verwendung als interner Standard wurden die Analyt-Matrix-Lösungen bei der Probenpräparation so mit der Jeffamine-Lösung versetzt, dass die Peaks des Standards zum Analyten Intensitätsverhältnisse von ca. 1:10 bis 2:1 erreichten.

Ergebnisse und Diskussion

Die positiv-Ionen MALDI-TOF-Spektren der vier Jeffamine (M-600, M-2005, D-400, D-230) zeigen durchweg intensive Peaks für $[M+H]^+$-Ionen, während $[M+Na]^+$ anders als bei nichtbasischen PEGs oder PPGs kaum auftreten. Der Trend zur Bildung anderer als [M+H]+-Ionen ist deshalb gering, weil die basische Endgruppe eine Protonierung auch durch wenig azide Matrizes ermöglicht. Unter den Jeffaminen erweist sich M-2005 geeignet, einen weiteren *m/z*-Bereich abzudecken. Außerdem liefert M-2005 ein übersichtliches Spektrum, in dem nur noch eine weitere Reihe von Peaks bei $[M+H–H_2O]^+$ auftritt.

Alle Jeffamine sind mit DCTB, CHCA und DHB kompatibel. Für die bei uns üblicherweise anfallen Proben ist DCTB eine besonders wichtige Matrix, da sie mit ihnen bei geringem Laserfluss intensive Signale und hohe Massenauflösung liefert. Polyalanin deckt zwar den Bereich *m/z* 1000–4000 in positiv- und negativ-Ionen-Modus ab [4], ist aber weder für DCTB geeignet, noch liefert es Spektren bei geringem Laserfluss.

Jeffamine M-2005 in DCTB zeigt im Vergleich zu PEG deutlichere Referenzpeaks deren Abstand von D(*m/z*) = 58 auch Interferenzen mit dem Analyten weniger wahrscheinlich werden lässt als D(*m/z*) = 44 bei PEG.

Das hier verwendete Jeffamine M-2005 entspricht dem im Nachtrag [3] zum ursprünglichen Artikel [2] publizierten Material. Mit Jeffamine M-2005 als internem Standard in DCTB-Präprationen von Analyten im Bereich von 300–1000 u lassen sich am Bruker Autoflex reproduzierbar Massengenauigkeiten von 3–5 ppm erzielen.

Eine Referenzmassenliste für Jeffamine M-2005 mit Werten von *m/z* 234 bis *m/z* 1220 ist erstellt und auf Wunsch auch elektronisch im Format für Bruker FlexControl verfügbar.

Neue Aspekte

Jeffamine M-2005 wird als neuer Massenstandard zur internen Kalibrierung für exakte Massenmessung in der MALDI-TOF-MS vorgestellt.

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ClCCA-Tetrazole: An alternative matrix for the analysis of low molecular weight compounds by MALDI-MS

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In recent years, the interest in MALDI-MS analysis of small molecules with a molecular mass below 1000 Da increased. Within this mass range the common MALDI matrix α-Cyano-4-hydroxycinnamic acid (CHCA) shows a strong matrix-background . Therefore some studies focused on the synthesis of CHCA-related compounds with similar characteristics but a different signal pattern to avoid interferences. One example, 4-Chloro-α-cyanocinnamic acid (ClCCA), is already established as MALDI matrix, but it only works with a laser wavelength of 337 nm.[1] In this study a new MALDI matrix related to ClCCA was tested, the carboxyl group was exchanged to a tetrazole ring with the aim of a bathochromic shift in the UV absorption and less matrix-background while maintaining the pH characteristics of ClCCA.

Experimenteller Teil

MALDI-MS analysis was performed with the Voyager STR Workstation (Applied Biosystems, Darmstadt, Germany). MALDI-MS/MS experiments were carried out with the Orbitrap XL LTQ Mass Analyzer (Thermo Fisher Scientific, Dreieich, Germany).

Solutions of ClCCA-Tetrazole, ClCCA and CHCA in 80 % acetonitrile with 0.01 % trifluoroacetic acid were prepared at the following concentrations: 1.5, 3 and 5 mg/mL. Standards of pharmaceutical compounds with a concentration of 100 ng/mL were prepared with the same solvent. MALDI spots were generated according to an optimized dried droplet preparation (DDP) protocol by spotting 1 µL of the matrix. After drying, 1 µL of the analyte was spotted. Additionally, the graphite supported preparation (GSP) protocol according to the work of Gorka *et a*l. was tested.[2]

Ergebnisse und Diskussion

In drug design 1H-tetrazoles are frequently used as bioisosteric modifications to replace a carboxylic group, because both have similar pKa and logP values but a different bioavailability.[3] This idea was adopted to create a matrix with similar characteristics to ClCCA. The calculated pKa of ClCCA-Tetrazole is 3.6 and therefore less acidic than CHCA (pKa=2.2) and ClCCA (pka=2.1). The UV absorption maximum measured in 80 % acetonitrile with 0.01 % trifluoracetic acid at a concentration of 30 µg/mL is λ=315 nm. A slight bathochromic shift compared to ClCCA, which shows a UV absorption maximum of λ=309 nm is observed. Additionally, the UV absorbance of ClCCA-Tetrazole at λ=337 nm is 43 % higher compared to ClCCA. ClCCA-Tetrazole showed a very homogenous crystallization at different concentration levels in the range of 1.5-5 mg/mL. At the first view its crystallization looked very similar to ClCCA and CHCA crystallization. But measurements with a scanning electron microscope exhibited differences. ClCCA-Tetrazole crystallized in homogenously distributed needles, while CHCA and ClCCA showed a platelet-like morphology. With GSP the crystallization behavior of all matrices changed completely. ClCCA and CHCA showed the already known rectangular crystals with a smaller size and a better distribution compared to the results of the common DDP.[2] In contrast the quality of ClCCA-Tetrazole crystallization deteriorated dramatically.

Signal intensities of fourteen pharmaceutical compounds were determined by MALDI-MS using ClCCA-Tetrazole, ClCCA and CHCA at different concentrations after DDP and GSP preparations. All ClCCA-Tetrazole spectra showed only few matrix signals. While GSP of ClCCA-Tetrazole was only advantageous for a small number of analytes, using DDP, nine out of fourteen analytes showed similar or higher signal intensities compared to ClCCA or CHCA. Therefore, we believe that ClCCA-Tetrazole is a good alternative MALDI matrix for small molecule analysis by MALDI-MS.

Neue Aspekte

Alternative MALDI matrix for small molecule analysis by MALDI-MS.

Referenzen

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Identification and characterization of N-acyl homoserine lactones by mass spectrometry

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In recent years, the processes which govern the communal behavior of humans, animals, plants with microbes have come to the focus of life sciences. The goal of this project was to develop analytical tools to identify molecules involved in interspecies communication, in particular of N-Acylhomoserine lactones (AHL), used by gram negative bacteria in quorum-sensing signaling. The developed methods for the analysis of AHL by means of LC-ESI MS/MS were applied to study the interactions of the fresh water polyp *Hydra* with its commensal microorganisms.

Experimenteller Teil

LC-ESI MS based methods were established focusing on the class of N-acyl homoserine lactone (AHL) autoinducers. To facilitate the identification of AHLs in biological samples, a library of AHL standards was created, which includes the spectral data (e.g. diagnostic fragments in MS/MS spectra) and retention-time information of 14 commercial AHL compounds. Using these data, the quorum-quenching activity of *Hydra vulgaris* polyps was analyzed and the resulting quorum-quenching product were identified. Furthermore, the product spectra of two AHL-synthases isolated from *Curvibacter*, the major colonizing bacterium of *Hydra*, were analyzed upon heterologous expression of the enzymes in *E. coli*.

Ergebnisse und Diskussion

The behavior of different AHL-derivatives in reversed phase chromatography was shown to be determined by the acyl-chain length and the oxidation state at the C_3 positions of the compounds. Retention times increased with the acyl-chain length. Among AHLs with the same acyl-chain length, 3O-AHL derivatives (with a carbonyl-group at C_3) eluted first, followed by 3OH-AHL compounds (with a hydroxy-group at C_3), while AHLs with aliphatic side-chains show the longest retention-times.

MS/MS fragmentation of AHL-compounds by CID and HCD on the Orbitrap Velos mass spectrometer revealed that, independent of the ion activation, all AHL produced a strong characteristic signal at m/z 102.055, corresponding to the singly charged homoserine lactone ring ion. This signal results from AHL fragmentation at the amide bond and is useful as a diagnostic ion for AHL. However, different ion activation methods and different substituents at the C_3-positon have a significant impact on fragmentation behavior resulting in characteristic fragmentation fingerprints.

Analysis of *Hydra* quorum-quenching experiments by MALDI-TOF MS and LC-ESI MS showed that *Hydra* polyps destroy a specific quorum-sensing signal by reducing the long-chained 3O-C_{10}-AHL to 3OH-C_{10}-AHL. Analysis of AHL-synthases from *Curvibacter*, revealed both enzymes to possess a very similar product spectrum, consisting exclusively of 3OH-AHLs. AHLs with different chain lengths were detected, including 3OH-C_{10}-HSL, 3OH-C_{12}-HSL and 3OH-C_{14}-HSL. The enzymes seem to specifically process acyl-ACP substrates carrying at minimum an acyl-chain length of C_{10}.

Together, these data reveal a novel quorum-quenching ability in *Hydra* and a very customized and interconnected quorum-quenching and quorum-sensing network in a host organism and its bacterial colonizer.

Neue Aspekte

- Discovery of a novel quorum-quenching mechanism in *Hydra*
- Characterization of the product spectrum of two AHL-synthase from *Curvibacter*

Combined Fast Mode and Polarity Switching for Analysis of a Range of Vitamins and Nutritional Supplements in a Single Injection

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Demand is increasing for high throughput LC-MS/MS analysis of chemically complex mixtures. For high throughput, HPLC or UPLC analysis of compounds such as vitamins and nutritional supplements, it is desirable to rapidly switch between ESI vs. APCI modes of ionization, positive and negative polarities, to facilitate analysis of diverse compounds within a single, fast injection. To do so requires switching times on the order of 10 ms, when switching between ionization mode or polarity, plus hardware which supports dual ESI and APCI functionality. A system so equipped would be capable of supporting multiple overlapping MRM transitions while maintaining a practically useful sampling rate for each MRM.

Experimenteller Teil

LC-MS/MS experiments were conducted on a mixture of vitamins and supplements such as 25OH Vitamin D3, α-Tocopherol, β-Carotene, creatinine, and co-enzyme Q10. This mixture was selected to span all combinations of ESI and APCI modes of ionization, positive and negative polarities, to demonstrate combined mode and polarity switching within a single LC injection. The experiments were conducted using a high performance dual source triple quadrupole mass spectrometer fitted with one ESI and one APCI probe. The sample inlet line from the Spark LC and autosampler was connected to a "T" which split the sample to provide continuous flow to each source probe. Total flow rate was 800 µL/min. with an injection volume of 15 µL.

Ergebnisse und Diskussion

The creatinine, vitamin D, and α-tocopherol essentially co-eluted, around 2 – 3 minutes, from the standard C-18 column. The co-enzyme Q10 eluted later, around 7 minutes. This was useful for demonstrating several capabilities of the system: The creatinine, vitamin D, and α-tocopherol MRM's overlapped in time, demonstrating fast switching between ESI+, APCI+, and ESI-modes of analysis. The co-enzyme Q10 MRM's overlapped with each other but not with the creatinine, vitamin D, and α-tocopherol, thereby demonstrating time optimization and fast switching between APCI- and ESI.

The capability for combined fast mode and polarity switching is an extremely valuable tool. It facilitates high throughput analysis of mixtures of chemically diverse compounds, by allowing the user to employ the ionization mode and polarity which is most suitable for each individual compound. Switching between positive and negative polarities, as well as between ESI and APCI modes of ionization, can be achieved within one injection.

Fast switching times lead to high sampling rates, so that large numbers of MRM's can be monitored simultaneously.

This capability can also increase efficiency for method development, and create flexibility for method optimization. Some compounds are clearly more amenable to one

specific ionization mode or polarity. Other compounds respond favourably to two or more different modes. Overlapping modes or polarities can efficiently determine which is most favourable, without the need for tedious repeat experiments. It can also allow the user to select the most favourable tradeoff for analyzing a particular mixture. For example, a molecule which is extremely fragile under ESI ionization, thus requiring a very low source and/or HSID temperature, could respond suitably to APCI ionization. The user can then select a higher ESI source temperature which might be more favourable for other components of the mixture.

Neue Aspekte

Combined Fast Mode and Polarity Switching in LC-MS/MS Analysis

Separation and identification of muscarine isomers

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Introduction

Many muscarine-containing fungi are considered to be toxic, often including fungi of the same genus, e.g. species of the Inocybe genus. However, reliable qualitative and quantitative data is often missing. In addition, only one of the eight possible muscarine isomers, (+)-muscarine (1), shows significant biological activity. [1,2,3] Thus, in order to make a viable assertion about the toxicity of a certain fungus, not only the determined concentration of muscarine but also the isomeric distribution needs to be considered.

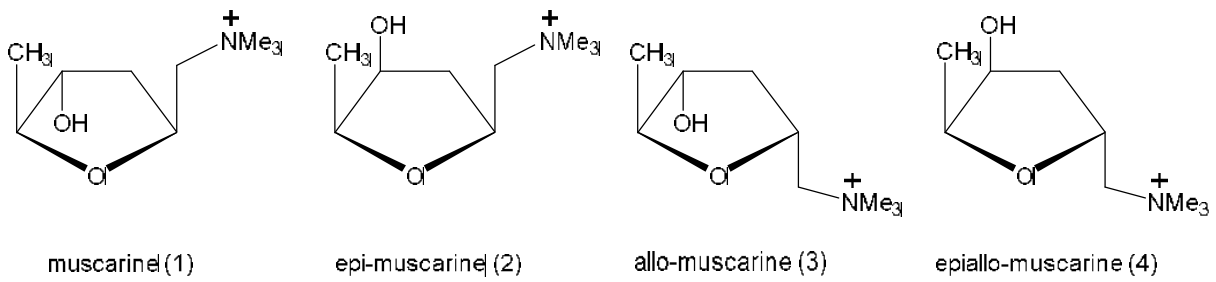

Figure 1: Diastereomers of muscarine.

Older investigations by Eugster et al., based upon the GC analysis of normuscarine obtained from the pyrolysis of muscarine chloride, showed significant fluctuations in the determined muscarine diastereomer ratio, even between collections of the same species. [4,5]

Experimental

GC-MS measurements were performed on a ThermoFinnigan Trace GC Ultra/DSQ GC-MS system. A Macherey-Nagel Optima 5 column (0.25 mm x 15 m) was used for separation. Temperature programs: a) GC-MS separation of normuscarine TMS derivates: 1 min 50°C, heating at 4°C/min up to 150°C, hold for 3 min. b) GC-MS separation of normuscarine MTPA derivates: 1 min 50°C, heating at 4°C/min up to 180°C, hold for 3 min.

LC-MS measurements were performed on an Agilent 1100 LC coupled to a Bruker Esquire-LC or a ThermoFinnigan LCQ Deca XP Plus MS. A Macherey-Nagel Nucleodur C18 ISIS column (3 mm x 250 mm x 5 µm) was used for separation. HPLC program: Isocratic, 90% H_2O (0.1% AcOH) / 10% MeCN.

Results and Discussion

Since much of the equipment and material used by Eugster et al. is no longer available today, our goal was the development of a method to separate, identify and (prospectively) quantify muscarine diastereomers and enantiomers from small

samples of fungi using current analytical equipment. To this end, muscarine-containing mushroom extracts were subjected to pyrolysis, yielding a mixture of normuscarine stereoisomers. To obtain diastereomeric separation, this mixture was derivatized with TMS and subjected to GC-MS analysis using an Optima 5 column, yielding baseline separation of (±)-normuscarine and (±)-epi-normuscarine. (±)-Epi-normuscarine could be distinguished from (±)-normuscarine by the lack of a characteristic fragment (m/z 141) in the EI mass spectrum. Normuscarine enantiomers could be separated after chiral derivatization with Mosher's reagent and GC-MS analysis on an Optima 5 column In this case, substance identification was done by comparison of retention times.

Separation of normuscarine diastereomers using LC has not been reported so far. We have developed a separation method for (±)-normuscarine and (±)-epi-normuscarine as TFA derivatives on a C18 ISIS column using an isocratic eluent and ESI-MS/MS detection.

Novel Aspects

GC-MS separation and identification of muscarine diastereomers and enantiomers, LC-MS separation and identification of muscarine diastereomers; ESI-MS/MS spectra of normuscarine.

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Keywords

Muscarine, normuscarine, diastereomeric separation, enantiomeric separation

Analysis of Pesticides in food product using SFE-SFC-MSMS

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1. Introduction

Conventionally, analysis of residual pesticides in foods has involved pesticide extraction by the QuEChERS method before analysis by LC/MS or GC/MS. However, it is time-consuming, and a large amount of organic solvent is used. Supercritical fluid extraction (SFE) that uses supercritical carbon dioxide as the extraction solvent provides good extraction efficiency, where the solvent is similar to a gas in terms of low viscosity and high diffusivity, and similar to a fluid in terms of high solubility. This allows for extraction within a short period of time. Hydrophilic pesticides can be extracted from a sample, as well as hydrophobic ones, by adding a modifier in the SFE process.

Supercritical fluid chromatography (SFC) is one of the separation techniques and it can separate numerous pesticides with a wide range of different polarities simultaneously. We also introduce an example of a GC-MS analysis of pesticides extracted from agricultural products using the Nexera UC off-line SFE system and the GCMS-TQ8040 (Shimadzu Corporation, Japan).

2. Materials and Methods

2.1. SFC-MS/MS: Analysis of a wide range of polarities of pesticides

System Shimadzu Nexera UC and LCMS-8050

SFC conditions
Column : Princeton 2-Ethylpyridine 150 x 4.6 mm, 5 µ
Mobile Phase (A) : CO_2
Modifier (B) : 16 mM $HCOONH_4$ in MeOH Gradient 0 %B to 90%B in 7 min
Flow rate : 3 mL/min
Back pressure : 15 MPa

LCMS 8050
Ionization method : Electro Spray Ionization (ESI)
Polality : Positive
Capillary Voltage : (2-4) kV
Nebulzing gas flow : 3 L/min
Heating gas flow : 10 L/min
Drying gas flow : 10 L/min
Desolvation Line T : 250 ºC
Heat block T : 400 ºC
Interface T : 300 ºC

2.2. SFE-SFC-MS/MS: Analysis of pesticide residues in food

System Shimadzu Nexera UC and LCMS-8050

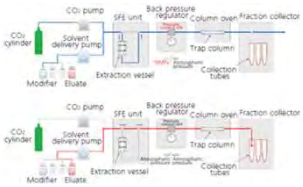
SFE conditions
Mobile Phase (A) : CO_2
Modifier (B) : 16 mM $HCOONH_4$ in MeOH
Flow rate : 5 mL / min.
Extraction : 0 - 1 min static mode (5 %B), 1 - 3 min dynamic mode (5 %B)
Extraction vessel T : 40 ºC
BPR : A: 14.8 MPa, B: 15 MPa (split rate: 3%)
Make-up : 16 mM $HCOONH_4$ in MeOH (0.4 mL/min)

SFC conditions
Column : Shim-pack UC-RP 5 µm (250 mm x 4.6 mm I.D.)
Mobile Phase (A) : CO_2
Modifier : 16 mM $HCOONH_4$ in MeOH
Flow rate : 3 mL / min.
Gradient program : 0 %B (0 min) → 10 %B (11 min) → 30 %B (14 min) → 40 %B (14.01-17 min)
Column T : 40 ºC
BPR : A: 15 MPa, B: 40 MPa
Make-up : 16 mM $HCOONH_4$ in MeOH (0.4 mL/min)

LCMS 8050
Ionization method : Electro Spray Ionization (ESI)
Polality : Positive and negative
Capillary Voltage : (2 - 4) kV
Nebulzing gas flow : 3 L/min
Heating gas flow : 10 L/min
Drying gas flow : 10 L/min
Desolvation Line T : 250 ºC
Heat block T : 400 ºC
Interface T : 300 ºC

2.3. SFE offline GC-MS/MS: Multi-residue analysis of organochlorine pesticides in food matrix

System Shimadzu Nexera UC and GCMS-8040



Offline SFE
Extraction vessel : 5 mL
Extraction solvent : CO_2 + methanol (5%)
Flow rate : 5 mL/min
Temperature : 60 ºC
Back Pressure : 15 MPa
Extraction time : 8 min (static extraction → dynamic extraction)

Trap condition
Trap Column : Shim-pack GIST C18 (50 x 4.6mm, 5 µm)
Temperature : 50 ºC

Recovery condition
Elution solvent : Acetone/Hexane = 50:50 v/v
Flow rate : 2 mL/min
Temperature : 60 ºC
Fraction time : 2 min (12 - 14 min)

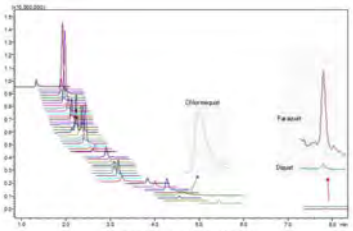
GCMS 8040
Column : Rxi-5 30 m × 0.25 mm ID, df = 0.25 µm
Sample injection : Splitless (250 ºC, Sampling time 1.00 min), high-pressure injection
Control mode : Linear velocity fixed (He, 47.2 cm/sec)
Oven temperature : 50ºC (1min) → (25 ºC/min) → 125 ºC → (10 ºC/min) → 300 ºC (15 min)
Injection volume : 1 µL
Ion source T : 200 ºC
Interface T : 250 ºC
Solvent cut time : 1.5 min
Detector voltage : 2 kV

3. Results

3.1. SFC-MS/MS: Analysis of a wide range of polarities of pesticides

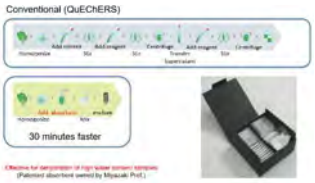
Pesticides having with different basic chemical structures, a wide range of polarities and molecular weight were chosen.
LOQ was between 0.1 and 10 µg/L

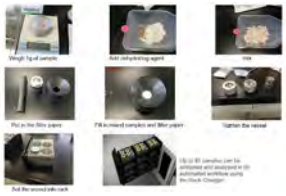
Compound	Log Kow	retention time (min)	R2	Range (µg/L)	LOD (µg/L)	LOQ (µg/L)
Aldicarb	1.1	2.1	0.987	1-250	1	1
Aldicarb sulfoxide	-0.6	2.9	0.991	0.1-250	<0.1	0.5
Aldicarb sulfone	-0.2	3.1	0.98	10-250	10	10
Atraton	2.7	2.0	0.991	0.5-250	0.1	0.5
Atrazindesethyl - desisopropyl	-0.11	4.7	0.988	1-250	1	5
Atrazine	2.61	2.4	0.991	0.5-100	0.1	0.5
Atrazine-desethyl	1.5	3.2	0.991	0.1-100	0.1	0.1
Chlormequat	-3.8	4.7	0.996	0.5-250	0.5	0.5
Chloroxuron	3.5	4.5	0.989	0.5-250	0.1	0.5
Chlorpyrifos-ethyl	5.3	2.0	0.983	5-250	1	5
Chlorpyrifos-methyl	4.3	2.0	0.978	1-250	0.5	1
Chlortoluron	2.4	3.8	0.991	5-250	5	5
Crimidine	1.31	2.5	0.983	5-250	5	5
Cyanazine	2.2	3.1	0.996	0.5-250	<0.1	0.5
Dimethoate	0.8	3.1	0.986	0.5-250	0.1	0.5
Diquat	-4.6	7.9	0.999	5-250	5	5
Diuron	2.7	4.6	0.991	0.5-250	<0.1	0.5
Fenthion	4.17	2.1	0.984	5-250	1	5
Fenuron	0.96	3.3	0.986	0.1-250	<0.1	0.1
Imidacloprid	0.8	5.5	0.99	0.5-250	<0.1	0.5
Isoproturon	2.9	3.2	0.991	0.5-250	0.1	0.5
Linuron	3.2	3.0	0.989	1-250	0.5	1
Malathion	2.4	1.9	0.999	0.1-250	0.1	0.1
Metamitron	0.7	4.0	0.99	0.5-250	<0.1	0.5
Metazachlor	2.38	2.0	0.992	0.1-100	<0.1	0.1
Methabenthiazuron	1.9	2.6	0.991	5-250	5	5
Methacrifos	1.9	1.3	0.982	5-250	5	5
Methiocarb	2.9	3.1	0.992	1-250	1	5
Metobromuron	2.4	2.5	0.989	1-250	<0.1	0.5
Metolachlor	2.9	1.9	0.992	1-250	0.1	1
Metribuzin	1.7	3.0	0.984	1-250	1	1
Monocrotophos	-0.2	2.4	0.991	0.1-250	<0.1	0.1
Monolinuron	2.3	2.4	0.992	0.5-250	0.5	1
Omethoate	-0.9	2.3	0.99	0.1-250	<0.1	0.1
Oxadiuron	4.8	1.9	0.995	0.1-250	0.1	0.5
Paraquat	-4.5	7.9	0.995	10-250	5	10
Phosphamidon	1.3	1.9	0.989	0.5-250	0.1	0.5
Pirimiphos-methyl	4.2	2.0	0.987	0.5-250	0.1	0.5
Prometryn	3.5	2.1	0.988	0.5-100	<0.1	0.5
Propazine	2.9	2.1	0.986	0.1-250	<0.1	0.1
Propham	2.6	2.1	0.912	10-250	5	10
Pymetrozine	-0.18	4.3	0.981	0.1-250	<0.1	0.1
Sebuthylazine	3.1	2.2	0.99	0.1-250	<0.1	0.1
Simazine	2.18	2.6	0.993	1-250	0.5	1
Terbutryn	3.2	2.2	0.996	0.1-250	<0.1	0.1
Terbutylazine	3.7	2.2	0.992	0.5-250	0.1	0.5



SFC Chromatogram at 50 µg/L

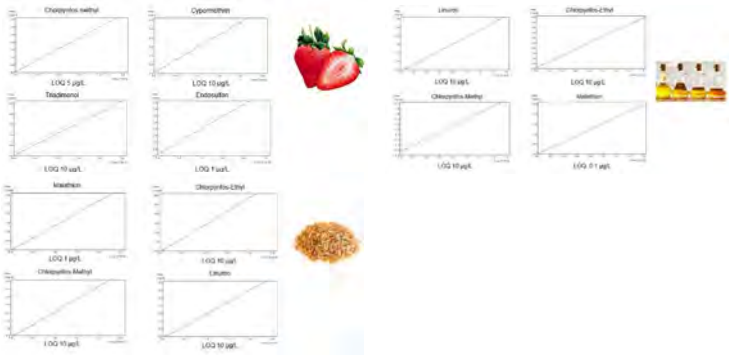
3.2. SFE-SFC-MS/MS: Analysis of pesticide residues in food





Example of calibration curve of extraction from strawberry, brown rice and oil

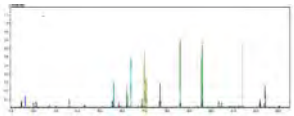
Different concentrations (1 to 200 µg/L) of a mix of almost 500 pesticides were spiked in brown rice, strawberry and oil.



3.3. SFE offline GC-MS/MS: Multi-residue analysis of organochlorine pesticides in food matrix

Calibration curves with standard solution (10 – 200 µg/L) in GCMS were created.
Linearity of response was demonstrated (r > 0.99).

Standard solution was spiked in **wheat** matrix (100 ng/g). After SFE offline extraction, the majority of compounds showed an accuracy between 80 to 125%



Chromatogram of organochlorines by GCMS after SFE offline extraction from wheat matrix

Compound	Accuracy (%)	%RSD (n=3)
Aldrin	70	0.7
BHC-alfa	73	6.2
BHC-beta	73	5.9
Bifenthrin	103	3.5
Chlordane-trans	76	1.6
Chlordane-cis	84	3.3
Chlorothalonil	28	6.4
Cypermethrin	101	3.9
DDD o,p	101	1.2
DDD p,p	56	2.9
DDE o,p	74	2.4
DDE p,p	79	2.3
DDT o,p	102	1.2
DDT p,p	96	11.3
Diclofop-methyl	23	3.4
Dieldrin	78	2.2
Endosulfan alfa	73	2.5
Endosulfan beta	95	0.7
Endrin	77	2.3
Fenvalerate I	84	4.7
HCB	71	1.2
Heptachlor	66	2.3
Heptachlor epoxide	88	3.0
Lindane	75	3.3
Methoxychlor	150	1.7
Mirex	103	5.4
Permethrin I	124	5.2
Permethrin II	119	7.5
Phenothrin	101	3.7

4. Conclusion

Supercritical Fluid Chromatography (SFC) is a hybrid of gas and liquid chromatography that combines some of the best features of each.
SFC can analyze different polarities of pesticides in the same method.
No need to use QuEChERS! SFE can be used online with SFC-MS and offline before GC-MS, Offline and online SFE can be used in the same batch.

Technische Universität München
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Validierung einer Stabilisotopenverdünnungsanalyse von Folaten in Lebensmitteln und Bestimmung des Folatgehaltes in Naturprodukten

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Einleitung

Die Vitamine der Folsäuregruppe gehören zu den wasserlöslichen Vitaminen und sind im Stoffwechsel vor allem bei der Übertragung von Methylgruppen beteiligt. Sie erfüllen essentielle Funktionen im Stoffwechsel der Aminosäuren und Nukleinsäuren (Selhub, 2002). Ein Folatmangel bei Frauen im gebärfähigen Alter gilt als Risikofaktor für den sogenannten Neuralrohrdefekt, einer Missbildung bei Neugeborenen (Czeizel & Dudas, 1992). Daneben kann eine Unterversorgung die Anfälligkeit von Herzkreislauferkrankungen (Robinson, 2000), Dickdarmkrebs (Caudill, 2004) und der Alzheimer Erkrankung (Snowdon, Tully, Smith, Riley, & Markesbery, 2000) erhöhen. Da die Folate vom menschlichen Körper nicht selbst gebildet werden können und somit mit der Nahrung zugeführt werden müssen ist es umso wichtiger, den Folatgehalt in Lebensmitteln mit einer sicheren Analytik zu quantifizieren. Es wurde eine sensitive Methode am LC-MS/MS 8050 gekoppelt mit einer Nexera X2 UHPLC für die Hauptvitamere in Lebensmitteln entwickelt und validiert. 5-Methyltetrahydrofolat (5-CH_3-H_4folat), 5-Formyltetrahydrofolat (5-CHO-H_4folat) und Tetrahydrofolat (H_4folat) wurden mittels Stabilisotopenverdünnungs-analyse unter Verwendung von ^{13}C-markierten Isotopen als interne Standards quantifiziert.

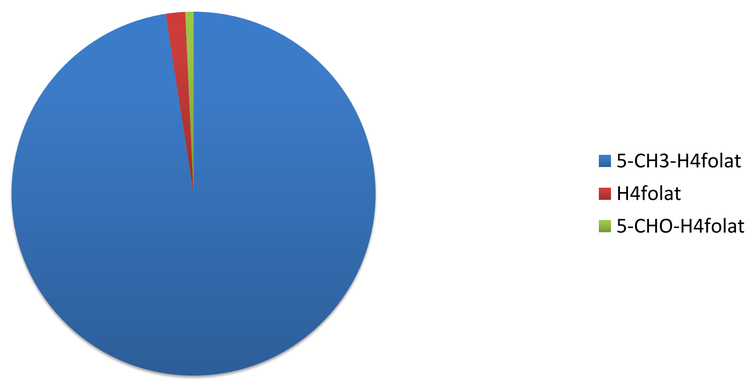
Ergebnisse

Die Chromatographie erfolgte auf einer Core-Shell C18-Säule, wodurch innerhalb von 5 min alle Analyten eluieren konnten (siehe Abbildung 1). Die Validierung der Methode ergab Nachweisgrenzen von 0,17 – 0.32 µg/100 g und Bestimmungsgrenzen von 0,51 – 0,93 µg/100 g. Die Extraktion zeigte gute Wiederfindungen im Bereich von 81,9 – 101,0 % und Wiederholpräzisionen mit relativen Standardabweichungen (RSD) von 3,04 – 5,06 % für alle Vitamere. Das Shimadzu 8050 Massenspektrometer zeigte Messpräzisionen mit RSD von 4,82 – 5,12 % (Tabelle 1 und 2). Bei der Quantifizierung natürlicher Folatquellen stellten sich Erdbeeren mit 104 ± 0.93 µg/100 g Gesamtfolat als gute, natürliche Folatquelle heraus. Der Gesamtfolatgehalt der Erdbeeren betrug 104 ± 0,93 µg/100 g. Das 5-CH_3-H_4folat war mit 101 µg/100 g das Hauptvitamer der Erdbeeren, während H_4folat und 5-CHO-H_4folat mit 1,78 und 0,76 µg/100 g nur in sehr geringen Mengen enthalten waren (siehe Abbildung 2).

Tabelle 1: Wiederfindung

Vitamer	Wiederfindung [%]
H_4-PteGlu	
Level 1	99,1 (10,1 µg/100g)
Level 2	99,4 (26,8 µg/100g)
Level 3	99,3 (90,4 µg/100g)
5-CH_3-H_4-PteGlu	
Level 1	96,7 (1,6 µg/100g)
Level 2	99,5 (42,7 µg/100g)
Level 3	101 (108 µg/100g)
5-CHO-H_4-PteGlu	
Level 1	81,9 (5,1 µg/100g)
Level 2	98,2 (15,6 µg/100g)
Level 3	96,7 (41 µg/100g)

Abbildung 2: Zusammensetzung der drei Hauptfolatvitamere in Erdbeeren



Material und Methoden

UHPLC-Methode

System	Shimadzu Nexera X2
Säule	Restek Raptor ARC18 2.7 µm 100 x 2 mm (@30 ºC)
Fließmittel	A Wasser + 0,1 % FA | B ACN + 0,1 % FA
Flussraten	0.4 $^{mL}/_{min}$
Injektionsvolumen	10 µL
Probentemperatur	+ 5 ºC

Mass Spectrometry

System	Shimadzu LCMS-8050
Ionisationsmodus	Heated ESI (HESI)
Temperaturen	
Heizblock |DL |Interface	400 ºC | 250 ºC | 300 ºC
Gasflüsse	
Drying Gas |HESI | Nebulizing Gas	10 $^{L}/_{min}$ | 10 $^{L}/_{min}$ | 3 $^{L}/_{min}$

Abbildung 1: LC-MS/MS Chromatogramme; obere Reihe: Responsemischungen, untere Reihe: Erdbeerprobe

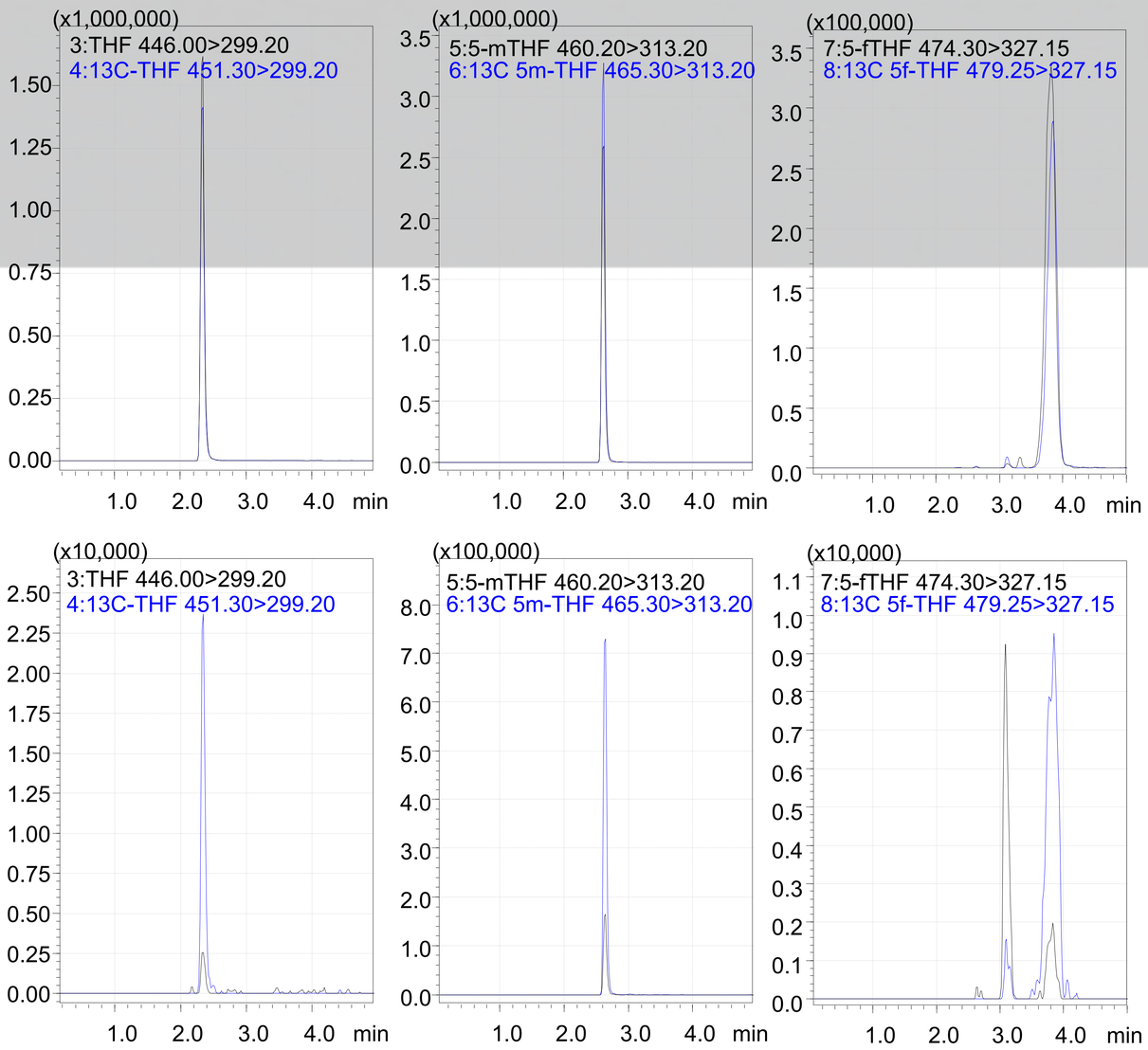


Tabelle 2: Präzision, Nachweis- und Bestimmungsgrenzen

Vitamer	Gerätepräzision RSD [%]	Wiederholpräzision RSD [%]	BG [µg/100g]	NWG [µg/100g]
H_4-PteGlu	5,12	5,06	0,76	0,25
5-CH_3-H_4-PteGlu	4,88	3,04	0,51	0,17
5-CHO-H_4-PteGlu	4,82	4,83	0,93	0,32

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Simultaneous quantitation and confirmation of about 500 pesticide residues in food extracts using LC-QTOF accurate mass spectrometry

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Fast and comprehensive full scan accurate mass screening and quantitation became an excellent tool in food control in particular if hundreds of pesticides have to be measured in a short time frame. Additionally to the high number of targets the technique takes advantage of unknown evaluation and retrospective analysis.

Experimenteller Teil

A set of 481 pesticides was selected. Matrix based dilution series (10 µg/kg – 2000 µg/kg, QuEChERS-extracts: tomato, summer squash, potato, orange) of the pesticide-mix were analyzed by an UHPLC connected to an impact II QTOF (Bruker) mass spectrometer using a 15 min gradient. Data acquisition is performed in alternating between full scan and bbCID all ion fragmentation mode.

Ergebnisse und Diskussion

Automatic data evaluation is performed using TASQ 1.1 (Bruker Daltonik GmbH), a dedicated software for target analysis screening and quantitation. For automated confident identification we use RT, accurate mass, isotopic pattern and up to 3 qualifier ions in full scan and 7 qualifier ions in bbCID. For tomato extract 454 of 481 pesticides or 94.3 % of the pesticides could be could be identified at 10 µg/kg and 98.9% at 50 µg/kg. For orange extract the numbers were 95.0% at 10 µg/kg and 98.9 at 50 µg/kg; for summer squash extract 91.3% at 10 µg/kg and 95.2% at 50 µg/kg; for potato 98.9% at 10 µg/kg and 99.6% at 50µg/kg.

Neue Aspekte

This study evaluates the performance achieved with a high performance QTOF, new software with a very high quality data base.

Parts-per-trillion level high-throughput quantitation of glyphosate, aminomethylphosponic acid (AMPA) and glufosinate in water samples by LC-MS/MS

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The global use of glyphosate, glufosinate and AMPA herbicides are strictly controlled by international regulations. We describe a method employing derivatization using 9-fluorenylmethyl chloroformate (FMOC) coupled with UHPLC-MS/MS tandem mass spectrometry to deliver a rapid and reliable method for the determination of glyphosate, AMPA and glufosinate in water samples.

Experimenteller Teil

Standards were spiked with glyphosate, AMPA and/or glufosinate. Incubate for 2 hours in Sodium tetraborate buffer and FMOC solutions. Phosphoric acid was added to stop the derivatization. Chromatographic gradient was between 2mM ammonium acetate and methanol, respectively, flowing at 0.4 mL min-1 through a C18 column. MS detector worked in MRM mode with heated-ESI negative ionization mode.

Ergebnisse und Diskussion

European guidelines require LC retention time of the in-matrix analyte must be within 2.5% of the retention time in the standard, and relative abundance of the MRM (SRM) transitions signals must be within 30% of the ratio obtained for the standards. Therefore, identification quality controls were tested using our method. The obtained results (especially LOQ and LOD) were low enough to meet the regulation about glyphosate and derivatives compounds in water analysis. The linearity and RSDRF of the calibration curves were between 5 and 20% and R2 0.999 respectively for the three compounds analyzed. S/N ratios of 10ppt points for all compounds were >= 10 and no significant carry over were detected following the 500ppt spiked sample. In summary, the method showed excellent linearity and sensitivity without exhibiting carryover whilst meeting the European Union regulations.

Neue Aspekte

Single method for multiple polar pesticides that is rapid, sensitive, low-cost and quantitative. Meets European MRL Guidelines.

Supercritical fluid extraction as a soil remediation method for removal of crude oil related contaminations, analyzed by FT Orbitrap MS

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Introduction

Soil is important for farming, forestry, animal husbandry and home to thousands of organisms. After over 200 years of industrialization 0.5 million contamination sites in Europe have been identified, with 3.5 million potentially contaminated sites. The annual cost for soil remediation was estimated at 2.4-17.3 billion euros. Polycyclic aromatic hydrocarbons (PAHs) from coking and manufactured gas plants and wood preservation sites are of great concern because of their carcinogenic, mutagenic and ecotoxicological effects.

Early results of supercritical fluid extraction (SFE) showed its potential for removal of PAHs and total petroleum hydrocarbons (TPH) from soil. By using High-field Orbitrap FTMS with its high mass resolution and accuracy this procedure is examined on a molecular level for the first time.

Experimental

Pure sand was spiked with diluted bitumen to yield a final concentration of 1g contaminant/1kg sand. The spiked sample was extracted using supercritical CO_2 ($scCO_2$) at 40 °C, 180 bar with a flow rate of 1, 2 and 4 mL/min for a time interval of 0-4 and 4-8 h, respectively. Afterwards remaining oil components from the sample were extracted using a Soxhlet extractor. The residue and extract fractions after SFE were compared with the original oil and a sample of direct Soxhlet extraction from the spiked sand.

Samples were analyzed by a research type Orbitrap Elite at a resolution of 960,000 (FWHM at *m/z* 400) using spectral stitching (30 Da windows with 5 Da overlap) by utilizing APPI/CI(+).

Results

With a combination of APPI and APCI a boarder range of PAHs, heterocyclic aromatic compounds (PAXHs, X=N, O, S) and also saturated nonpolar components can be examined at the same time.

Extraction of soil is a method that allows easy remediation of soil from industrial areas. Using supercritical conditions with CO_2 as solvent is a method that is tested against standard extraction methods, such as Soxhlet extraction.

When using a Soxhlet extraction of spiked sand a recovery of 84% can be achieved with no significant differences found between mass spectra of the original oil and extract. This indicates that the lost mass during extraction consisted mainly of volatile compounds.

Here we show the results comparing Soxhlet extraction with SFC extraction of the residue and extract (0-4 h and 4-8 h) and compare them with the original crude oil. The data reveal that pure hydrocarbons (HC), sulfur and nitrogen containing PAHs can be extracted over the whole mass range by $scCO_2$; whereas the extraction efficiency of oxidized PAXHs was lower. Components with lower carbon number and with double bond equivalent (DBE) smaller than 30 were more easily to be extracted; although after 8 h the extraction was still not complete, most dominant components were extracted in 4 h already.

Different $scCO_2$ flow rates influence the extraction efficiency more than the composition. HC, S_{1-4}, and N classes with low to medium DBE values could be extracted by all three flow rates. But with increasing flow rate the intensity of extracted components decreased. The intensity of each signal in the sample extracted at a flow rate of 4 mL/min was only 40-50% of the intensity in the sample performed at 1 mL/min. This reveals that the lower flow rate shifted the equilibrium more to the mobile phase and therefore favored the extraction.

New aspects

SFE of crude oil related contaminations in soil was investigated using FTMS on a molecular level for the first time.

Keywords

Fouier transform Orbitrap mass spectrometry, supercritical fluid extraction, crude oil, soil remediation

Title: Methodological aspects of mass spectrometric detection for profiling ambient VOCs with thermodesorption-GCMS

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Introduction

Profiling of VOCs from environmental and biological samples is still very challenging due to the broad range of volatility, different chemical classes and polarities of their components. VOCs are commonly collected from gaseous samples by adsorption to materials such as the polymer Tenax TA, then released by thermal desorption, and analyzed by GC-MS. However, Tenax TA is quite expensive so that efficient alternatives are searched for that could replace the material. In combination with mass spectrometry, however, these materials need to provide a particularly low background apart from general requirements such as speed and efficiency of sampling and subsequent complete release upon thermal desorption.

Experimental Section

We investigated if and under which conditions the polymer XAD-2 could provide a broader coverage for (semi)polar VOCs during gas-phase sampling compared to Tenax TA. A standard mixture of 57 compounds covering a wide range of volatility (bp. 20 - 256 °C) and different chemical classes was introduced by liquid spiking into in-house packed sorbent tubes with one of the two porous polymers, Tenax TA or XAD-2. Sensitivity and repeatability of compound quantitation were analyzed by a *GCMS-TQ8040* system composed of a thermal desorption unit TD-20 and a gas chromatograph *GC-2010 Plus* coupled to a triple quadrupole mass spectrometer (Shimadzu Europe GmbH, Duisburg, Germany).

Results and Discussion

A higher flow rate of 1.15 L/min could be achieved with XAD-2 compared to the lower flow rate of 0.69 L/min for Tenax TA while recovery and repeatability of the volatiles were satisfactory with both, pre-packed and in-house packed. We obtained less than 20 % relative standard deviation, RSD (12 % for Tenax TA and 15 % for XAD-2). Approximately 30% of the compounds exhibited a better LOD with Tenax, all others had similar ranges for quantitation, i.e. between 0.02 and 2000 ng ± <20 % RSD and $R^2 > 0.99$ for both sorbent materials. The general intensity pattern obtained with a comprehensive standard mix of 57 compounds was very similar between XAD-2 and Tenax TA.

However, huge blank signals of at least twelve artifact compounds (sum of intensities for the twelve detected compounds, approximately 9.7% of the TIC) were detected from XAD-2 during thermal desorption above 220 °C. Apart from the severe degradation of the adsorption material itself, these artifacts led to a higher background noise, aging of the adsorption material and GC column and

accumulating contamination in the MS system. To avoid the presence of these artifacts, lower temperatures were tested in the first stage of the thermal desorption system. As a result, the signal intensity of the thermal breakdown products dropped dramatically compared with the signal at the highest tested temperature (250 °C), with only little effect on the signal intensity for the compound mix (< 15 % signal reduction) when decreasing the desorption temperature by 30 or 60 K.

In conclusion, the large-surface porous XAD-2 material indeed can be regarded as alternative to Tenax TA in terms of compound selectivity and recovery.

Novel Aspects

In GC-MS analysis, XAD-2 can be recommended as an alternative to Tenax TA for VOC sampling followed by thermal desorption.

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Keywords
VOCs, thermal desorption, GC-MS, XAD-2

Fenton based oxidation of crude oil in supercritical CO_2

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Introduction

Crude oil contaminated environment is not habitable for neither human beings nor the micro-habitants. Efforts for the removal of PAHs from contaminated soil focus on either their oxidation to CO_2 and H_2O or their transformation into non-toxic, biodegradable products. Here, the Fenton reaction can be used for those advanced oxidation processes. Performing the reaction in supercritical CO_2 ($scCO_2$) has many advantages over organic solvents such as nontoxicity, non-flammability and easy removal of the solvent. For the analysis of complex mixtures like crude oil, ultrahigh-resolution mass spectrometry is a powerful method to get a comprehensive characterization of the oxidized species obtained during the reaction.

Experimental

The Fenton oxidation was set up under batch and under supercritical conditions. In both conditions, heavy crude oil was mixed with deionized water, perchloric acid, H_2O_2 and $FeSO_4$. The reaction under batch was stirring for 24 h at room temperature. For the Fenton experiment in $scCO_2$, the autoclave with the reaction mixture was filled with compressed CO_2 and heated up to the desired temperature of 50 °C.

Mass spectrometric analysis was performed using a research-type Orbitrap Elite mass spectrometer (Thermo Fisher, Bremen, Germany), operating at a resolving power of using 480,000 (FWHM at m/z 400) either ESI or a combination of APPI and APCI.

Results and discussion

The difficulty to remove complex mixtures of polyaromatic hydrocarbons (PAH) and polyaromatic heterocycles (PAXH) from contaminated soil lies in the fact that the number of

different compounds is very high making the mixture extremely complex. One method that allows degrading such complex PAH and PAXH mixtures is the Fenton chemistry. In this reaction, hydrogen peroxide in the presence of a Fe-catalyst is being used to oxidize the aromatic cores. Combining the reaction with the green chemistry approach of low solvent consumption the reaction was carried out under $scCO_2$ conditions.

For the understanding of the degradation ultrahigh resolution mass spectrometry is the method of choice. First results show that a broad variety of compounds are oxidized and degraded. The analysis of the products by ESI(-)-FTMS allows the detection of high oxygen containing compounds while the combination of APCI and APPI leads to detection of less polar hydrocarbons and aromatic heterocyclic compounds that have not yet reacted under the applied conditions.

The results show that sulfur containing polycyclic aromatic hydrocarbons (PAHs) are more easily oxidized than the pure hydrocarbons. Especially, the abundances of oxidized sulfur species are increased more after the Fenton reaction under $scCO_2$ conditions.

Comparing the Fenton reaction under supercritical and atmospheric conditions to the unreacted crude oil shows that the abundances of low oxygen containing compounds (O_{1-4}) are increased. Furthermore, a variety of high oxygen containing compounds (O up to 8) is newly created and appears after the reaction. Fenton reaction in $scCO_2$ has a positive influence on the oxidation efficiency, because as the APCI and APPI results show, higher abundances of oxygen containing PAHs were observed under supercritical conditions.

New aspects

Fenton reaction in supercritical CO_2 is a promising reaction for the artificial degradation of crude oil.

Keywords

Crude oil, Fenton reaction, supercritical CO_2, Fourier transform Orbitrap mass spectrometry

Effect of temperature on crude oil fouling under inert and oxygenated conditions and subsequent analysis by HRMS

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Introduction (112/120)

One of the main problems in the petroleum industry is the deposition of unwanted material on the heat exchange equipment. Although crude oil contains only a small percentage of heteroatom-containing compounds such as nitrogen, oxygen, and sulfur, they are responsible for adverse effects (coke formation, fouling, corrosion, catalyst poisoning, and environmental pollution). The chemical complexity of crude oil in combination with its instability leads to different chemical transformations that till now are poorly understood. In addition, various parameters such as temperature influence these processes. High resolution mass spectrometry enables understanding the reaction mechanisms of crude oil, as well as the role of the various parameters play to them on a molecular level.

Experimental (78/120)

A lab build reactor was used for testing a light Arabian crude oil. The samples were heated at temperatures ranging from 150°C to 450°C under oxygen and argon conditions. Samples were collected and measured after 3 days. For mass analysis a research-type Orbitrap Elite was used. Spectra were collected in SIM mode with a mass resolution of 480000 (FWHM at *m/z* 400, 1.5s transient). ESI positive and negative was used with a potential of 4kV and 3.5kV respectively.

Results (217/300)

The results obtained under oxygen and argon conditions at different temperatures are presented. In positive mode measurements under oxygen, N_1 class was the dominating one for all the temperatures, followed by the NO_x classes. With the increase of the temperature there was an increase of these classes. S_1 class was found only in the unreacted crude oil, which indicates the highly reactivity of sulfur under oxygen conditions. In addition, OS class was detected in the unreacted oil as well as at the temperature of 150°C and 250°C. When running the reaction under inert conditions sulfur containing compounds were present throughout the whole procedure. At 350°C

and 450°C formation of coke was observed. Formation of radicals was observed under ESI(+) with $HC^{\cdot}$ radicals to show the highest abundance. The maximum number of carbon and DBE detected under oxygen conditions were 69 and 54 respectively. Under argon conditions the values were lower. Finally, under ESI(-) the O_x classes were the most abundant, with the number of the oxygen containing compounds to reach up to O_8. Radicals of O_1 class, up to O_5 class were observed in both cases. The biggest difference of the O_x species compared to the unreacted one, can be seen after O_4 class, where the abundance of the species after heating is almost 3 times higher.

Novel Aspects (17/20)

The fouling behavior of crude oil under different conditions is investigated on a molecular level by HRMS.

Investigations on the photolysis of sulfamethoxazole

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The removal of micropollutants from surface waters is a topic of growing awareness. Not all xenobiotics are sufficiently removed by municipal wastewater treatment plants. As a result, additional disinfection steps such as ozonation or direct photolysis utilizing UV light are investigated. Many of these procedures are already well elucidated regarding degradation efficiency or energy costs but only few studies deal with the identification of formed transformation products and their toxicity.

In the present study, the photolytic degradation of the frequently used antibiotic sulfamethoxazole (SMX) using polychromatic UV light is investigated focusing on the identification and characterization of formed transformation products via high performance liquid chromatography coupled to electrospray ionization mass spectrometry (HPLC-ESI-MS). The oxidative degradation of SMX using direct photolysis with UV light has been realized with a high-pressure mercury lamp (250 W) emitting light in the range of 220-500 nm. The SMX solutions were adjusted to pH 3 and pH 8 using a phosphate buffer to study the pH dependency of product generation.

The photolytic degradation of the antibiotic sulfamethoxazole in aqueous solutions has been investigated to characterize transformation products. In total, more than 20 different mass-to-charge ratios could be found, ten of which have been published before. It was shown that the pH value has a great impact on how SMX is degraded and what transformation products are formed. Most obvious is the greatly reduced degradation time of SMX at pH 3. To degrade SMX to a similar level, the photolysis needs 18 min at pH 8 whereas it takes only 4 min at pH 3. Additionally, the main transformation product varies depending on the used pH value. While the photolysis of SMX at pH 3 mainly leads to an isomerization of SMX itself, at pH 8, a broader variety of main products is formed.

The pH and irradiation time dependency of the UV degradation of sulfamethoxazole were elucidated by ESI-MS regarding formed transformation products.

Analyzing self-assembly of Ebola virus nucleoprotein with native mass spectrometry

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KEYWORDS

Native MS, Ebola virus, nucleoprotein, self-assembly

INTRODUCTION

Ebola virus (EBOV) forms helical filaments containing the nucleoprotein (NP) as essential component. NP_{1-450} includes domains for self-assembly and RNA-binding.[1] Therein, a motif ($NP_{313-321}$) is present that is highly conserved among *Filoviridae*.[2] Identifying the motif's function, its role in self-assembly by means of native mass spectrometry is the aim of this project. In order to monitor the reversible oligomerization it is required to produce recombinant, soluble protein. Of further interest is how RNA and EBOV proteins affect the process. By creating $NP_{313-321}$ mutants it can be determined if the motif is crucial for the assembly, and hence for infectivity. The strong conservation among *Filoviridae* gives occasion to perform comparative experiments to examine if the idea is applicable to other viruses.

MATERIALS & METHODS

EBOV nucleoprotein is expressed in *E. coli* BL21(DE3)pLysS cells. Recombinant proteins are purified by immobilized metal ion affinity chromatography and size-exclusion chromatography (SEC). Expression and purification are evaluated by SDS-PAGE and Western Blot. Native mass spectrometry is used to identify NP monomers and assemblies, furthermore to run interaction studies with binding partners, e.g. RNA and viral proteins. Besides, NP assemblies are observed by transmission electron microscopy (TEM).

RESULTS

Purity of recombinant EBOV nucleoprotein was confirmed by SDS-PAGE and Western Blot. Despite being purified by different chromatography methods, UV absorbance at 260 nm indicated that nucleic acids were present. Strong nuclease treatment combined with sonication lightly decreased absorbance at 260 nm. During size-exclusion chromatography the retention time of the NP-containing fraction was lower than expected, suggesting presence of oligomers with noticeably larger hydrodynamic radius than the monomer. Protein samples observed by electron microscopy showed occurrence of ring particles with a size of 30-40 nm in diameter. Monomeric Nucleoprotein was detected by native mass spectrometry in buffer with low ionic strength. Peaks representing a pentameric formation of the protein were dominant in a large range of buffer salt concentrations.

Conclusion

EBOV nucleoprotein is known to have a role in replication. It encapsidates the viral genome. Thus, NP contains RNA binding domains. Presence of nucleic acids was found to be persistent during our experiments indicating a strong binding of bacterial RNA. Since NP's main function is the formation of the nucleocapsid, the protein contains domains for NP-NP interactions which control the process of self-assembly. Results of SEC and TEM show that a specific oligomer, a ring structure, seems to be an intermediate structure during the formation of the full nucleocapsid. The stoichiometric composition of NP that was found to be most prevalent in native mass spectrometry measurements was a pentamer. It was detected at physiological salt concentration, whereas the monomer only could be observed in buffers with very low ionic strength, indicating that lower salt concentrations prevent self-assembly and therefore the protein's function. Next, the assembly and importance of the conserved residues will be studied in more detail.

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New aspects

Native MS measurements of self-assembling Ebola virus nucleoprotein display protein complex formation.

Native mass spectrometry analysis of norovirus - glycan mimetics interaction

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co-authors,

Introduction:

Human noroviruses (HuNoV) are non-enveloped RNA viruses belonging to the Caliciviridae family and being the main cause of viral gastroenteritis. From crystallographic structures, it is apparent that norovirus capsid protein protruding (P) domain binds to glycans on the cell to mediate cell attachment [3]. Owing to "soft" electrospray ionization technique, native mass spectrometry (MS) enables characterization of non-covalent protein-glycan ligand interactions in a single experiment without the need for titrations [4]. Whereas binding affinity to individual glycans is low, multivalency on the cell surface supposedly results on strong avidity. To investigate the impact of multivalency on viral cell entry, binding of multivalent glycan mimetics, linear oligomer chains with monosaccharides attached [5], to P domains is analyzed by native MS.

Experiments:

Different combinations of glycan mimetics and HuNoV strains were tested in native MS. Multivalent glycan mimetics resembling the high density of glycans on cell surfaces were used for binding to P domain to characterize binding affinity and avidity. The results are compared to binding of natural monovalent glycan ligands to elucidate how multivalency impacts cell attachment.

Results:

The results will elucidate binding profiles and dissociation constants of distinct noroviruses to glycan mimetics. This will also explore whether glycan mimetics have potential as antivirals. Preliminary data show similar affinity for the first binding event from single sugar to multi-valent glycan mimetics indicating that further adaptions are required to study avidity. An introduction to native MS for non-covalent interaction study and latest results for the next generations of glycan mimetics will be presented.

Keywords:

Native mass spectrometry, human noroviruses, glycan-mimetics, P domain, binding interactions.

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From Salty to Salt-free: Monitoring the Salt-dependent Dissoziation of the Membrane Protein Complex GCD in a Single Experiment

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NaCl-concentration and ionic strength of the buffer solution play an important role for the stability of many proteins and protein complexes. Even with the advancements of native-MS in recent years, high NaCl-concentrations still present a major problem for the nanoESI-methods typically employed for the analysis of protein complexes due to signal oppression and peak broadening.

Here we present an alternative approach using LILBID-MS to successfully analyze the membrane protein complex GCD[1] (Glutaconyl-CoA-Decarboxylase) from *Clostridium symbiosum* from a buffer solution containing 100 mmol NaCl. This approach can also be used to gradually reduce the NaCl-concentration during the measurement, allowing us to monitor the disaggregation of the complex to obtain signals of the individual sub-units, revealing their salt-dependent stability.

Experimenteller Teil

LILBID-MS spectra were obtained on an in-house-build re-TOF instrument. In the LILBID-source, micro droplets of the sample solution are introduced into the ion source with a frequency of 10 Hz and are irradiated with mid-IR laser pulses at a wavelength of 2.94 µm. The subsequent explosive evaporation of the micro droplets leads to the release of the sample ions.

nanoESI-MS Spectra were measured on a Synapt G2-S Q-TOF instrument. The sample was sprayed using Pd/Pt-coated borosilicate needles prepared in-house.

For LILBID spectra a solution of 10 µmol/L GCD in a buffer containing of 50 mmol Tris, 100 mmol NaCl and 0.02 % DDM was used. For nanoESI, this solution was buffer exchanged to 100 mmol Ammonium acetate and 0.02% DDM.

Ergebnisse und Diskussion

The stability of the GCD membrane protein complex is strongly dependent on a sufficient NaCl-concentration of about 100 mmol in the sample solution. This makes it impossible to obtain mass spectra of the intact complex when using nanoESI as the ionization method for the determination of the complex stoichiometry. In contrast to ESI, the LILBID mechanism relies on the release of pre-charged ions from the evaporating micro droplet and leads to significantly lower charge states. It is also much less sensitive with regards to buffer conditions, especially the NaCl-concentraion of the solution.[2]

Using LILBID-MS it was possible to obtain signals, albeit broad and in relatively small intensity, of the intact protein complex at a NaCl-concentration of 100 mmol. This enabled us to determine the stoichiometry of GCD to be 2:2:2:2 with regard to the 4 individual sub-units A, B, C and D.

When the sample is loaded from the front opening into the water-filled capillary of the micro droplet generator, the NaCl-concentration of the sample solution decreases over the time of the measurement. This is due to the big size difference between the protein and the salt ions. These ions migrate much faster back into the capillary, thus leading to a constantly diminishing NaCl-concentration as the measurement proceeds, while the protein concentration stays almost constant. In the case of GCD, this effect expresses itself in the increase of the highest detected charge state of the protein complex and also in the occurrence of signals of incomplete, dissociating protein sub-complexes and ultimately the detection of single sub-units.

In the comparative nanoESI experiments only signals of the individual sub-units from a desalted solution could be seen.

Neue Aspekte

Monitoring the salt-dependent disaggregation of a membrane protein complex in a single native-MS experiment.

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Studying viral capsid glycan interaction with native MS

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Glycans are carbohydrate structures that cover cell surfaces and are generally known as multivalent attachment factors. Specific variants of glycans, oligosaccharides such as histo-blood group antigens (HBGAs) and glycosaminoglycans are used as receptors by many viruses. However, the mechanism of host protein glycan interactions in viral attachment and cell entry is not completely understood. In this work three viruses are targeted, namely Noroviruses (NoV), Merkel Cell Polyomaviruses (MCPyV) and Human Papillomaviruses (HPV). Capsids of these viruses can be recombinantly produced. They have a major and a minor capsid protein that self-assemble into virus like particles (VLPs). These VLPs are greatly differing in their size, ranging from about 10 MDa to 20 MDa.

We are establishing native MS for the investigations of whole viral capsids binding to glycans. To study these high-mass capsids, the purification and buffer exchange require optimization. Capsid stability and characterization tests are performed as described by Shoemaker et al. 2010 [1]. Buffer conditions are varied, differing in ionic strength and pH. Subsequently, the impact of glycan-binding and altered capsid stability can be described by a population shift.

NoVs are well known for their interaction with glycans like HBGAs. Preliminary work of our group as well as STD NMR titration data could show that HBGA-binding to NoV of the GII.4 Saga strain is a multi-step process. Furthermore, native MS data reveals four instead of two binding sites per P-dimer [2].
Data from stability tests on VLPs of the NoV strain GII.17 Kawasaki show a different behavior compared to the Norwalk strain (genogroup I) capsid described by Shoemaker et al. [1]. The Kawasaki strain is not as sensitive towards ammonium acetate concentrations and pH values.

The presentation illustrates challenges and approaches when studying high mass particles with native MS.

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Keywords

Native mass spectrometry (MS), viral cell entry, glycan binding, structural changes

Profiles of glycated amino acid adducts in the protein hydrolyzates of pea (*Pisum sativum*) seeds subjected to accelerated ageing

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Introduction

Protein glycation is referred to the reaction of lysyl and arginyl residues with reducing sugars and dicarbonyl products of their degradation. Resulting advanced glycation end products (AGEs) represent a heterogenic group of modified amino acid residues, accumulating during thermal processing and prolonged storage of foods. In human organism, dietary AGEs trigger development of subclinical information and atherosclerosis. Hence, prolonged storage of protein-rich plant-derived foods might represent a health thread for consumers. Therefore, the contents of AGEs in plant materials need to be determined. However, the required methods are still not established. We propose the sample preparation strategy for exhaustive hydrolysis of total plant protein samples and apply it to characterization of AGE profiles in ageing pea seeds by UHPLC-ESI-MS.

Method

Yellow-colored pea seeds were subjected to accelerated aging by treatment at 45°C and 86% relative humidity during 3 days and 5 days [1]. The total protein fraction was isolated from the pea seeds, (n = 3) by phenol extraction [2]. The protein pellets were reconstituted in an aqueous detergent solution and subjected to exhaustive enzymatic hydrolysis [3]. The completeness of hydrolysis was verified by SDS-PAGE, before detergent was removed by RP-SPE, and derivatized with N^2-(5-fluoro-2,4-dinitrophenyl)-L-valine amide (L-FDVA) was performed [4]. The analysis relied on RP-UHPLC-ESI-LTQ-Orbitrap-MS. The data were processed by the Compound Discoverer Software (Thermo Fisher Scientific), and differentially abundant amino acid adducts were identified by exact mass and ESI-MS^n analysis.

Results and discussion

As glycation products are relatively labile and readily degrade under high temperatures and acidic pH, only few AGEs can be reliably quantified under these conditions. Therefore, exhaustive enzymatic hydrolysis was performed. However, as the total protein preparation contained high amounts of highly-hydrophobic membrane proteins, it could not be quantitatively dissolved in aqueous phosphate buffer, required for the digestion. Therefore, the pellets were reconstituted in presence of 10% sodium dodecyl sulfate (SDS) and 20-fold diluted with phosphate-buffered saline (pH 7.5) to obtain a 0.5% solution, not disturbing enzymatic activity. The hydrolysis was performed as described by Glomb and co-workers, using successive treatment with pronase E, proteinase K, and carboxypeptidase Y for 24, 18 (both 37° C), and 24 h (25° C), respectively [3]. After enzymatic digestion, the detergent was successfully retained on SPE cartridges, as could be assessed by flow injection MS analysis. The eluates were lyophilized, reconstituted in 20% (*v/v*) aq. acetonitrile, derivatized with L-FDVA [4], and analyzed by RP-UHPLC-ESI-LTQ-MS. The profiles represented the majority of the previously characterized AGEs. The pattern of AGEs dominated with N^{ε}-(carboxymethyl)lysine (CML), N^{ε}-(carboxyethyl)lysine (CEL), N^{δ}-(carboxymethyl)arginine (CMA), N^{δ}-(carboxyethyl)arginine (CEA), argpyrimidine, and methylglyoxal-derived hydroimidazolone (MG-H), which could be reliably characterized by their tandem mass spectrometric fragmentation patterns.

Significance

In this study, for the first time the full profiles of plant-derived protein glycated adducts were obtained

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Analysis of 1,2,3,4-diepoxybutane induced DNA-histone cross-links by mass spectrometry

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Introduction

DNA replication and transcription are the fundamental processes of cellular maintenance and survival. They are mainly mediated by transient DNA-protein interactions. Therefore, detection and identification of these interactions is crucial for a better understanding of cellular DNA-protein complexes. Mass-spectrometry-based cross-linking approaches have been used to detect and identify DNA-protein interactions. However, low yields of cross-linking products impede faithful MS/MS-based identification of cross-links. In order to analyze DNA-protein interactions, cross-links can be generated in various ways e.g. by radiation or exposure to chemical cross-linking reagents. Here, we used the highly reactive electrophile 1,2,3,4-diepoxybutane (DEB) that is capable of inducing DNA-protein cross-links, and thus may increase cross-linking yields and facilitate identification of cross-linking sites.

Experimental setup

Core histone H3 and linker histone H1.4 were produced recombinantly. Two different dsDNA sequences of 21bp, and 187bp in length were incubated with H3 or H1.4 in presence of the cross-linking agent DEB. After quenching of the reaction DNA and protein were hydrolyzed enzymatically. Subsequently, non-cross-linked DNA was removed by C18 spin columns. Cross-linked peptides were enriched by TiO_2 affinity chromatography and measured on a Tribrid Orbitrap mass spectrometer (Fusion Lumos, Thermo Scientific). Spectra were analyzed using the RNP^{xl} pipeline of OpenMS, generating potential precursor variants used for manual MS/MS spectra annotation [Kramer *et al.,* 2014].

Results and Discussion

In a proof-of-principle experiment histones H3 and H1.4 were incubated with DNA in presence of DEB. So far, we identified guanine nucleobase as the prime target site cross-linking mainly lysine residues to DNA. This is in line with reported cross-linking of guanine to DEB [Tretyakova *et al*., 2015]. Additionally, cross-links to thymine were identified, however, the individual cross-linking sites have not been mapped yet to a crystal structure.

Besides protein-DNA cross-linking, DEB proved to be an effective protein-protein cross-linking agent as analyzed by gel-shift analysis and mass spectrometry.

In summary, our identified cross-linking sites are supported by published data. Our approach demonstrates that chemical cross-linking reagents such as DEB are promising candidates to extent the current spectrum of cross-linking techniques and thus contribute to our understanding of transient DNA-protein interactions.

Novel aspects

Mass spectral analysis provides deeper insights into the cross-linking potential of chemical reagents for protein-DNA interactions.

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Precise quantification of HIV proteins by isotope dilution mass spectrometry (ID-MS) for applications in HIV diagnostics

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Organisationen: 1: Physikalisch-Technische Bundesanstalt; 2: Technische Universität Braunschweig

Einleitung

In therapy of HIV infected patients, decision of therapy success is depending on reliably monitoring virus concentration in blood, the HIV viral load. The development of molecular approaches (quantitative and digital PCR) in the last decades enables the detection of low levels of pathogens, but challenges remain regarding comparability and standardization of measurements due to the lack of traceable reference standards and methodologies (*1, 2*). Therefore, the idea is to establish an independent approach to virus quantification, which is based on measuring viral proteins. ID-MS as an established primary method for protein quantification would be a powerful tool. The analytical method can be applicable to viral load quantifications in HIV samples, but also to calculations of the HIV maturation status.

Experimenteller Teil

For HIV quantification by ID-MS, the bottom-up proteomics approach is used to generate specific peptide fingerprints by tryptic cleavages of proteins. Peptides with high HIV sequence conservation were selected. Isotopically labeled analogues (^{15}N and ^{13}C amino acids) are added at the beginning of sample preparation as internal standard. The peptide mixture is separated by two chromatographic steps (cation exchange, reverse phase) and finally, peptides are identified and quantified by Orbitrap Elite based ESI-LC-MS/MS analysis.

Ergebnisse und Diskussion

Specific peptides from the HIV Gag-Polyprotein are present throughout the whole HIV maturation process and can thus be used to deduce the total HIV viral load. During the maturation process, the Gag-polyprotein is cleaved into the single proteins matrix, capsid, spacer 1, nucleocapsid, spacer 2 and p6 peptide by the viral protease (*3*). Thus, peptides which overlap two single proteins of the Gag-Polyprotein are cleaved during the maturation and hence are specific for immature virus particles. Combining both parameters shall allow the calculation of the viral maturation level.

The analytical ID-MS method for the quantification of such peptides is developed and optimized using recombinant HIV proteins as the capsid and nucleocapsid protein. In the next step, the method will be applied to HIV samples which currently are produced under BSL3 conditions.

Neue Aspekte

Development of an analytical ID-MS method for precise and traceable HIV protein quantification

Referenzen

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Stichwörter
human immunodeficiency virus, ID-MS, viral load

Themen
Proteine und Proteomics, Organische Massenspektrometrie

Title:

Investigating on-plate digestion of proteins with regard to trypsin activity and oxidation

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Einleitung (max. 120 Wörter)

Recently published methods for on-plate digestion [1,2] show that this method is a useful alternative to in-solution digestion for protein identification and characterization. In particular, the implementation of reduction and alkylation on the MALDI-target led to a reduction in analysis time and to fast protein identifications[1]. During experiments for method development, we observed oxidation on peptides and had less satisfying results with high reagent amounts. Here we evaluate some problems, which may occur during sample preparation and digestion. We investigated common reagents and detergents for their inhibition potential on trypsin, their effect on lipophilic peptides in MALDI-MS analysis and the effect on oxidation during the sample preparation steps and possible solutions to these particular problems.

Experimenteller Teil (max. 120 Wörter)

Material

Bovine insulin and serum albumin were diluted to 10 µM and 1 µM, respectively. Dithiothreitol, IAA, laurylmaltoside, deoxycholate and octylglycoside were diluted to different concentrations for MS- and UV-Vis measurements. Iron(II)sulfate and Ferene S were diluted to a final concentration of 80 µM and 10 mM, respectively. CHCA-matrix was used in a concentration of 3 mg/mL.

Sample preparation and mass spectrometry

A SunDigest System (*SunChrom, Friedrichsdorf, Germany*) was used as described in [1] for on-plate reduction, alkylation and digestion. All mass spectra were recorded on a MALDI-Orbitrap XL LTQ *(Thermo Fisher Scientific, Dreieich, Germany).*

UV-Vis measurements

The measurements of the trypsin activity and the iron(II) oxidation were carried on a Tecan M300 infinite spectrophotometer. Wavelengths were adjusted according to [3,4].

Ergebnisse und Diskussion (max. 300 Wörter)

Reduction and Alkylation on-plate

We investigated reduction and alkylation carried out directly on the MALDI-sample plate and compared it to in-solution reduction and alkylation. For this purpose insulin was used, which

can be reduced and alkylated without the need of digestion and BSA to optimize the sample preparation prior to digestion. Results showed that a higher DTT amount and higher IAA amount lead to a higher reduction and alkylation extent for insulin, but above 20 mg/mL DTT and 30 mg/mL negative effects on the matrix crystallization were observed. Reduction, alkylation and digestion of BSA each showed an optimal reagent concentration range and were used to define a standard workflow.

Effects of different detergents on the insulin spectra

To enhance the data quality for lipophilic proteins, we tested different detergents as additives for tryptic digestion. For MALDI-MS PMF spectra laurylmaltoside showed the strongest signal improvement for lipophilic peptides as expected due to its lowest critical micelle concentration of all tested detergents. A negative influence of the detergents on the crystallization of the matrix was not observed, on the contrary laurylmaltoside formed more homogenous preparations compared to CHCA alone.

Effects of sample preparation reagents on the trypsin activity

DTT, IAA and all used detergents, except DOC, were investigated for their potential to inhibit trypsin. Laurylmaltoside and octylglycoside apparently enhance the efficiency of trypsin, most likely due to a higher substrate solubility. IAA doesn't affect trypsin, but DTT has a strong effect and decreasie the activity to 50%.

Effects of sample preparation reagents on protein oxidation

To evaluate oxidations on protein we used iron(II) sulfate as a surrogate parameter for oxidation. Investigations showed that higher temperature lead to a higher oxidation extent using the on-plate approach. Different additives such as detergents and reagents were tested, DTT prevents oxidation successfully.

Neue Aspekte (max. 2)

1. Investigation of oxidation and trypsin inhibition during on-plate digestion

2. Identifying potential trypsin inhibitors and enhancers for lipophilic peptide analysis

Referenzen (max. 5)

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Stichwörter (max. 5)

On-plate digestion

On-plate reduction and alkylation

Oxidation

Method development

MALDI-MS

Applying a Proteoform profiling method for neurological disorder biomarker discovery operations

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Proteomics investigations in biofluids have revealed that most proteins are present as a variety of proteoforms (combination of isoforms, proteolytic processing & PTM results). Measuring the intact mass of proteins by MS has the advantage to provide information on the relative amount of the different proteoforms. We have applied this approach for neurodegenerative diseases study.

Experimenteller Teil

Cerebrospinal fluids (CSF) samples from 30 patients already diagnosed with Alzheimer's disease (AD), and controls were analyzed using an Impact II (Bruker Daltonics) with both a nanoflow and a normal-flow LC-MS analysis. After statistical analysis, Scheduled Precursor Lists have been used to fragment the proteoforms of interest and characterize them with BioTools (Bruker Daltonics).

Ergebnisse und Diskussion

The overlap of masses detected with the nanoflow and high-flow approaches was below 15%, and the mass accuracy obtained was below 2 ppm. Statistical analyses have been performed on more than 5000 compounds reproducibly detected in patient samples. MS results have been correlated with clinical data, to end up with a first list of more than 70 differentially regulated compounds. Those fragmented biomarker candidate have then been identified and characterized. The results confirmed that several isoforms of APP, clusterin or transthyretin were differentially expressed in the CSF of AD patients, when compared to the CSF of the other groups.

Moreover, several isoforms of chromogranin/secretogranin (synaptic biomarker family) were detected, some showing a differential expression in the three clinical groups assayed.

Neue Aspekte

Neurological biomarkers identification and characterization based on TDCP approach allowed to identify differentially regulated proteoforms in CSF.

CHARACTERIZATION OF CARBOHYDRATE BINDING SITES IN GALECTINS BY PROTEOLYTIC AFFINITY - MASS SPECTROMETRY

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Galectins are a family of proteins defined by their binding specificity for β-galactose-containing glycoconjugates and share primary structural homology in their carbohydrate-recognition domains (CRDs). They are involved in crucial cellular processes such as cell-cell adhesion, cell migration, cell development and differentiation, chemotaxis and apoptosis. Together with another class of animal lectins, the C-type lectins, they exert various functions within innate immunity mechanisms. Beyond being involved in crucial cellular processes, galactosides inspired new lead compounds for glycan-directed drug design can be derived from lectins. The elucidation and availability of peptides mimicking the target specificity of the galectin would enable tests for clinical applicability, either to elicit favourable effects such as antitumor signalling or interfere with premalignant processes.

Experimenteller Teil

Proteolytic extraction mass-spectrometry was used to identify the ligand-contacting peptides. Proteolytic digestion of galectin-3 was performed with a trypsin/galectin ratio of 1:100 and the proteolytic mixture bound to the affinity matrix (lactosylated Sepharose 4B) in phosphate-buffered saline. Unbound material was then removed by thorough washing with buffer to ensure that even weakly bound material would be removed, prior to competitive elution with buffer solution containing 0.3 M lactose. The eluted epitope fraction was collected, desalted and characterized by ESI-IonTrap mass spectrometry.

Ergebnisse und Diskussion

The mass spectrometric analysis of the last washing faction yielded no peptides, and analysis of the elution fraction yielded two distinct tryptic peptides. Together, these two peptides harbored the key amino acids in contact with the ligand, thus representing the bioactive sequence parts of galectin-3.

This method allowed rapid molecular determination of carbohydrate binding sites in galectins with high sensitivity and low requirements in sample purity.

Neue Aspekte

Affinity MS is a promising tool to investigate protein - carbohydrate interaction.

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Comparison of label free quantification methods for proteomics

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For the quantification of proteins in complex biological samples, there are many different Liquid Chromatography-Mass Spectrometry (LC-MS) based methods. Two label free quantification methods are Data Dependent Acquisition with the MaxQuant software (DDA) [1] and Data Independent Acquisition (DIA) [2]. DDA is based on the area under the curve (AUC) of the individual intact precursor ions (MS1 level). In contrast, DIA quantification is done based on the AUC of fragment ions (MS2 level). In this study, both methods were compared by performing an analysis of an androgen-repressed metastatic prostate cancer cell line (ARCaP cell line).

Experimenteller Teil

ARCaP cells were homogenized and a protein extract recovered. The protein sample was digested with trypsin and desalted. Both DDA and DIA experiments were run as biological triplicates on a Dionex UltiMate 3000 nanoUPLC (Thermo) coupled to a Q Exactive (Thermo) mass spectrometer. The data from DDA runs was processed by MaxQuant, post-analysis and statistics were done by Perseus. For the DIA experiment, the library was generated first, then the DIA runs were done. Library generation and DIA data processing was done by Spectronaut software (Biognosys), post-analysis and statistics by Perseus.

Ergebnisse und Diskussion

The DDA and DIA experiment were compared in terms of identified proteins, reproducibility and quantification. Filtering criteria were chosen conservatively and as similar as possible for the post analysis due to the differences in the output files from the processing software. At the moment, Spectronaut doesn't work with unique peptides, a common filtering criteria for MaxQuant data. The number of identified proteins in DIA was 893, in DDA 740. The number of missing values (MV) on peptide level was lower and the reproducibility better with DIA too. Through the DIA experiment, the average of MVs was 163 per run and the median coefficient of variation (CV) 11.4 %. The corresponding MVs in DDA were 1777 per run, the median CV 24.6 %. For peptides identified in both experiments, the AUCs were compared. They showed a correlation of 47.8 %. The DIA experimental setup is more time consuming. With a good working LC-MS setup and good software algorithms for the data analysis, the invested time in the DIA setup for this experiment have shown to result in a better performance.

Neue Aspekte

Comparison between two different label free quantification methods.

Referenzen

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Abstract für DGMS Kiel 2017

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Titel des Beitrags:

Structural Insights into Retinal Guanylyl Cyclase/GCAP-2 Interaction by Cross-linking and Mass Spectrometry

Einleitung:

Retinal guanylyl cyclases (ROS-GC 1 and 2) are membrane proteins with a modular structure [2] that are regulated via the intracellular site by guanylyl cyclase-activating proteins (GCAPs) in dependency of the intracellular Ca^{2+} concentrations [1]. However, the exact mechanisms of how GCAPs activate their target proteins are still not fully characterized as exclusively structures of non-activating Ca^{2+}-bound GCAP-1 and -2 are available. In a previous study, cross-linking MS-analysis between GCAP-2 and a short peptide derived from catalytic domain of ROS-GC1 had pointed to a well-defined structure of the GCAP-2/GC peptide complex in calcium-bound state [3]. To gain deeper insight into the ROS-GC activation by GCAP-2, we use the complete catalytic subdomain of ROS-GC1 for cross-linking/MS analysis.

Experimenteller Teil:

The structural investigation of the ROS-GC1 homodimer and the ROS-GC1/GCAP-2 complex was performed via a chemical cross-linking/MS approach. For the cross-linking experiments, the catalytic ROS-GC domain with *C*-terminal extension was expressed in *E.coli* and purified by affinity chromatography via the HLT-tag and by size-exclusion chromatography. The enzymatic activity of the catalytic ROS-GC domain was monitored measuring the turnover rate of GTP to cGMP by LC/SRM (selected reaction monitoring)-MS. For the structural investigation of the ROS-GC1 homodimer and ROS-GC1/GCAP-2 complex, various cross-linkers bridging a range of distances were employed. Proteolyzed reaction mixtures were analyzed by nano-HPLC/nano-ESI-MS/MS (Ultimate RSLC 3000 coupled to an Orbitrap Fusion mass spectrometer). Also, photo-methionine was incorporated into GCAP-2 to gain complementary structural information by photo-cross-linking (UV-A irradiation).

Ergebnisse und Diskussion:

After expression in *E.coli* and purification of the catalytic ROS-GC1 domain, the enzymatic turnover of GTP to cGMP was monitored by LC-SRM-MS. Initial structural insights into the ROS-GC homodimer were obtained by the amine-reactive deuterated cross-linker bissulfosuccinimidylglutarate (BS^2G-D_0/D_4) and our *in-house* developed MS/MS cleavable urea-based cross-linker BuUrBu. To discriminate between intra- and inter-molecular cross-links within the ROS-GC homodimer, non-labeled and fully ^{15}N-labeled ROS-GC were applied in a 1:1 ratio. Cross-linked products between two ROS-GC monomers have so far only been identified in the *C*-terminal region of the catalytic domain, but the respective cross-links have not been validated yet. For gaining insights into the protein interface between the catalytic ROS-GC domain and its binding partner GCAP-2, different cross-linking strategies were pursued. Various amine-, sulfhydryl-, carboxyl-, and photo-reactive cross-linkers bridging a range of distances were employed, which however did not result in the identification of defined cross-links between the both binding partners. Future cross-linking experiments will focus on optimizing the reaction conditions and eventually on using a smaller ROS-GC domain.

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Neue Aspekte:

For the first time, we use the isolated catalytic subdomain of ROS-GC to unravel the mechanisms of ROS-GC activation by GCAP-2.

Themen: Proteine & Proteomics

Stichworte: Retinal guanylyl cyclase, cross-linking, GCAP, mass spectrometry

Kategorie: cross-linking, structure analysis

Synthesis of Isotope-Labeled Derivatives of the MS/MS-Cleavable Urea-Cross-Linker: Synthesis and Evaluation of Reactivity for Effective Protein Structure Analysis

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Introduction

Chemical cross-linking (XL) in combination with mass spectrometry (MS) has matured into a valuable alternative strategy for deriving structural information of proteins and protein assemblies where NMR and X-ray crystallography reach their limits.

Several amine reactive homobifunctional *N*-hydroxysuccinimide (NHS) active ester reagents have been developed. A number of them provide MS/MS labile covalent bonds allowing sensitive collision-induced dissociation (CID)-analysis. One of these cross-linkers is the well studied "urea-linker"[1] which has been successfully employed in a number of cross-linking studies.

To further confirm and simplify the identification of cross-linked species from a complex peptide mixture, a combination of isotope-labeled and non-labeled cross-linker was tested. Therefore, deuterium and ^{18}O-labeled derivatives of the urea-linker were synthesized.

Experimental section

An exhaustively deuterium-labeled variant ("D_{12}-Urea XL") as well as a doubly ^{18}O-labeled ("^{18}O-Urea-XL") variant of the urea linker were synthesized and probed for chemical cross-linking.

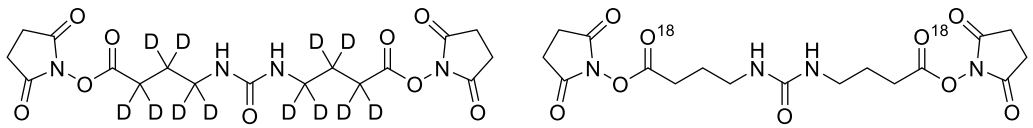

Fig.1: Left: D_{12}-Urea-XL, **Right:** ^{18}O-Urea-XL.

The deuterium-labeled variant was synthesized following standard protocols using 4-aminbutyric acid-2,2,3,3,4,4-D_6 to form the free diacid.[1] The ^{18}O-variant was synthesized using the non-labeled free acid in a TFA (1%) catalyzed ^{16}O-^{18}O exchange in ^{18}O enriched water.[2] Both derivatives were activated for effective amine-reactivity by introducing an NHS-ester moiety. Initial XL-experiments were performed with β-lactoglobulin and BSA as test proteins. Cross-linked proteins were digested with trypsin and the peptide mixtures were subjected to nano HPLC/nano-ESI-MS/MS on an Orbitrap Fusion Tribrid instrument (Thermo Fisher Scientific). Cross-links were identified with the MeroX 1.5.1 software.[3]

Results and Discussion

Synthesis of the D_{12} derivative of the urea-linker resulted in moderate product yields. The acid catalyzed ^{16}O-^{18}O exchange was nearly quantitative after 16 days.

Initial cross-linking experiments were performed following standard protocols, linking β-lactoglobulin and bovine serum albumin (BSA) at different pH-values, with different cross-linker concentrations followed by in-solution or in-gel digestion. Data analysis documents a comparable cross-linking efficiency of the isotope labeled and non-labeled derivatives.

Experiments to integrate the D_{12} linker in our automated workflow[4] and thereby facilitating the identification of cross-linked species are ongoing. First TMD-(target mass difference)-triggered experiments, with a mixture of D_{12}-Urea-XL and D_0-Urea-XL linked peptides, documented the feasibility to identify cross-linked species by automated TMD-triggering.

D_0/D_{12} XL-product ion pairs were used to determine the retention time shift between the cross-linker species during RP (reverse phase)-HPLC analysis (< +/- 0.5 min). We suggest that the influence of the urea moiety on the elution behavior is superior to the influence of the deuterium labels, facilitating an automated identification of cross-linked species. As such, data processing with MeroX 1.5.1[3] was possible with all isotope labeled derivatives.

Further experiments with the isotope labeled urea-linker reagents to establish an automated workflow are subject of ongoing investigations.

New Aspects

Novel isotope-labeled variants of the urea-linker are tested for effective and automated chemical cross-linking, showing promising features.

Keywords

Peptide Cross-Linking, (CID)-ESI-MS/MS, Protein structure analysis.

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Mass Spectrometry-Based Interaction Studies of the *N*-Terminus of the Formate Channel FocA from *Escherichia coli*

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Introduction

The formate channel A (FocA) belongs to the formate-nitrite transporter (FNT) family and translocates formate across the membrane in a bidirectional fashion. Detailed structural information is available from X-ray studies indicating that FocA forms a homopentamer within the bacterial inner membrane [1, 2]. However, there is no clear mechanistic understanding on how formate passage is controlled through the FocA channel. Previous studies had indicated that FocA's termini are involved in the regulation of formate transport [3]. In order to validate this hypothesis we have screened for interaction partners of the *N*-terminus of *E. coli* FocA using cross-linking/mass spectrometry (MS). Our goal is to elucidate how protein-binding partners of FocA influence formate transport.

Experimental

The coding sequence for the *N*-terminus of FocA was fused to the malE-gene, which encodes maltose-binding protein (MBP). The N-FocA-MBP fusion protein was produced in *E. coli* BL21 (DE3) and purified. For identification of protein interaction partners, the fusion protein was incubated with anaerobically grown *E. coli* K12 cell-free lysate. Chemical cross-linking was carried out with the amine-reactive MS/MS-cleavable cross-linker (BuUrBu). Proteins cross-linked to the *N*-terminus of FocA were affinity-purified via the MBP tag and cross-linked products were analyzed after enzymatic digestion with trypsin using nano-HPLC/nano-ESI-MS/MS (Ultimate 3000 RSLC coupled to Orbitrap Fusion Tribrid mass spectrometer, Thermo Fisher Scientific). Protein identification was conducted with Proteome Discoverer 2.1 (Thermo Fisher Scientific); quantification was performed by label-free quantification using MaxQuant.

Results/Discussion

We are planning to use a combined affinity purification and cross-linking/MS approach to determine protein interaction partners with the *N*-terminus of FocA. As a first step, FocA was expressed with a C-terminal MBP tag for an affinity-enrichment of FocA/protein complexes after the cross-linking reaction. However, our cross-linking studies have so far been hampered by significant amounts of endogenous *E. coli* maltose-binding protein. Therefore, we are currently exploring the use of alternative affintiy tags for the enrichment of cross-linked FocA/protein complexes.

Novel Aspects

Use of a combined affinity purification and cross-linking/MS approach to elucidate protein interaction partners of the *N*-terminus of FocA.

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A versatile method to extract, modify, enrich and digest proteomic samples directly from cell lysates

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Einleitung (120/61)

Methods developed previously within our workgroup to mimic Arg-C digests [1] relied on commercially available cell lysates of E. Coli or model proteins. Here, we compare different lysis methods of human cell lines, in combination with the enrichment and quantitative modification of proteomes on magnetic beads, to maximize extraction and identifications, while minimizing effort, time consumption and costs.

Experimenteller Teil (122/131)

HEK 293T and E. Coli cultures were harvested and washed with PBS buffer.
3 aliquots of the cell pellet were lysed with Bugbuster® buffer and proteins were precipitated from the supernatant with acetone and resuspended in 100mM TEAB.
3 aliquots underwent lysis with 8M Urea and Lysonase™ and the precipitate discarded after centrifugation. Protein concentrations were determined via BCA-Assay and equalized.

10µl BcMag™ magnetic silica beads (Bioclone Inc) suspension was incubated with 100µg of protein sample for 1h, reduced with DTT (45min, 57°C) and alkylated IAA (45min, RT, light exclusion). The supernatant was discarded and the beads were washed twice with 100mM TEAB. Propionylation of lysine residues was performed as described by Golghalyani et al[1]. Samples were digested with trypsin and analyzed via LC-MS/MS.

Ergebnisse (124/300)

Of the evaluated lysis protocols the single-step urea/Lysonase™ lysis not only allows for direct incubation of the beads and is thus time efficient, it also increases the amount of proteins immobilized to over 90% as determined via BCA Assay and moreover provides up to 500 more identified proteins over lysis methods that include an additional acetone-precipitation step.
The protein extraction via beads is thus not impaired by harsh buffers like 8M Urea, 6M Guanidine-HCl and organic solvents.
In total we could identify up to 3051 unique proteins from the HEK 293T samples utilizing Arg-C-like digest by masking trypsin cleavage sites at lysines by their propionylation[1]. Further optimization might include pre-fractioning the samples orthogonal to their behavior in RP-HPLC environment. Moreover an overall comparison with a standard tryptic digestion protocol will be carried out.

[1] V. Goghalyani, ArgC-like digestion: Complementary or alternative to tryptic digestion? (Journal of Proteome Research – 2017 in press)

Investigation of Q-TOF instruments advantages for label-free proteome analysis

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The capacity of detecting very accurately and reproducibly differences between peptide and protein ratios in different samples is key to understand the proteome dynamic. This study illustrates how the UHR-QTOF's combination of intra-spectral dynamic range, reduced space charge effects, speed and spray stability translate into label-free proteomics enhanced performances.

Experimenteller Teil

Label-free quantitative performance of an impact II -instrument (Bruker Daltonik GmbH) was investigated using a 1:2 mixture of human cell line and yeast proteomes. A nanoLC was coupled to the Q-TOF via a CaptiveSpray ionization source. Peptides were separated using a 90 min gradient and analyzed with a Self-Adapting LCMS/MS method. Data have been analyzed applying the MaxLFQ algorithm.

Ergebnisse und Diskussion

The quantity of human cell line proteome was kept constant for both samples. The yeast proteome was spiked in two different amounts resulting in a 2-fold increase for all yeast proteins. Consequently, we created a highly complex sample set with the possibility to detect fold changes over the complete dynamic range. Results showed a high reproducibility between technical replicates (R2 ~ 0.99). Nearly all (~95%) of the non-changing human proteins had CV values below 20% and roughly 70% even below 10%. The overall difference between changing and non-changing population was 1.9, i.e. very close to the theoretical one of 2 and thereby representing excellent accuracy of the evaluated Q-TOF instrument for label-free proteomics. The data showed that the instrument can easily cover 4 orders of magnitude of dynamic range in the sample for identification as well as for quantitation.

Neue Aspekte

In-depth investigation of advantages of Q-TOF technology for label-free proteomics by mixing complex proteomes.

Development of a protein interaction networks in synaptic vesicles using cross-linking and mass spectrometry

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Synaptic vesicles (SVs) are small organelles in the presynaptic terminal of neurons responsible for storage of neurotransmitters. During signal transduction, induced by an action potential, SVs migrate to the presynaptic side of the nerve terminal and fuse with the plasma membrane (exocytosis). Thereby the neurotransmitters are released into the synaptic cleft. One SV cycle therefore includes neurotransmitter import, exocytosis, including the neurotransmitter release as well as vesicle recycling. SVs are densely packed with proteins most of which are identified to-date. Current SV models assume a random distribution of the proteins in the membrane, but there is evidence of functionally active protein complexes. We set out to identify these protein complexes and their protein interactions using cross-linking strategies.

Experimenteller Teil

Intact SVs were purified from rat brain according to standard protocols [e.g. 1]. We used bis(sulfosuccinimidyl) suberate (BS3), ruthenium(II) tris-bipyridyl dication ($[RU(II)bpy])_3^{2+}$), 4-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-methylmorpholinium chloride (DMTMM) in the presence or absence of adipic acid dihydrazide (ADH) for cross-linking of SV proteins. Cross-linked proteins were (i) separated by SDS-PAGE and digested in-gel with trypsin or (ii) digested in-solution and pre-fractionated by gel filtration. Generated peptides were analysed by LC-MSMS on a Q-Exactive Plus Hybrid Quadrupole-Orbitrap or an Orbitrap Fusion Tribrid mass spectrometer (Thermo Scientific). Raw data were converted into mgfs using pxtract software tool and potential cross-links were identified using pLink software [2]. Spectra of potential cross-links were validated manually. Protein networks were visualised using XVis web server [3].

Ergebnisse und Diskussion

SVs were purified from rat brain following established protocols. Major proteins of SVs were then identified by LC-MS/MS and database searching. These proteins include Synapsin, Synaptotagmin, Synaptophysin, Syntaxin, Synaptogyrin, Synaptobrevin, VGlut and subunits of the V-ATPase.

To identify protein interactions in SVs, we followed different cross-linking strategies targeting basic or acidic amino acid residues: (i) First, we employed BS3 cross-linker, which specifically reacts with lysine side chains. (ii) We also used DMTMM in the presence or absence of ADH to covalently link acidic (presence of ADH) or acidic and basic (absence of ADH) amino acids. (iii) We also employed photolysis of $[RU(II)bpy])_3^{2+}$ in the presence of ammonium persulfate to link tyrosine residues with tyrosine, histidine, threonine, serine or lysine residues, respectively. While BS3 and ADH introduced flexible linkers into the cross-linked proteins, the other two strategies cause zero-length covalent linkage between the proteins.

Applied in this way, we obtained many protein interactions from BS3 cross-linking reactions. Cross-linking with DMTMM revealed fewer protein interactions, mostly within the proteins (intra-protein cross-links). However, few inter-protein interactions were also identified, mostly between subunits of the V-ATPase. Zero-length cross-linking revealed only few protein interactions (intra- und inter-protein) suggesting that most of the SV protein complexes are rather flexible.

Chemical cross-linking proved as a valuable tool to study protein interactions and revealed first interaction networks in synaptic vesicles. These networks contain many protein interactions with Synaptobrevin which plays a central role in complex formation. Local networks, for instance between Synaptophysin, Synapsin and subunit a of the V-ATPase, were also observed. Surprinsingly, almost no interactions were observed with Synaptotagmin, one of the major vesicle components. However, numerous intra-protein cross-links were identified between calcium binding domains suggesting a remarkable flexibility of this calcium sensor.

Neue Aspekte

Our cross-linking studies revealed first insights into the protein interaction networks in synaptic vesicles.

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Phthalate metabolites MEHP and MEOHP but not the phthalate DEHP itself bind and activate the PPARγ

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Abstract – The metabolic syndrome, accompanied by obesity, insulin resistance, type 2 diabetes mellitus and cardiovascular diseases became a growing problem over the last years. One of the key regulators of the connected pathways is the peroxisome proliferator-activated receptor gamma (PPARγ) with its endogenous ligand, the 15-deoxy-delta-12,14-prostaglandin J_2 (15Δ-PGJ_2). It has been reported that exposure to one of the most frequently occurring phthalates, the di-(2-ethylhexyl)phthalate (DEHP), causes adverse effects on glucose homeostasis and insulin sensitivity [1, 2]. This could be linked to the structural similarity of DEHP and its main metabolites mono(2-ethylhexyl)phthalate (MEHP) and mono(2-ethyl-5-oxohexyl)phthalate (MEOHP) to the 15Δ-PGJ_2. To test this hypothesis, interactions of DEHP, MEHP and MEOHP with PPARγ were tested by hydrogen-deuterium exchange (HDX) mass spectrometry (MS).

The HDX-MS experiments were carried out using a fully automated system (Waters Corporation). To obtain data for the free deuterated PPARγ as reference, the protein was incubated for 60 s in D2O and the deuteration was quenched subsequently. For the investigation of the interactions, the PPARγ was preincubated with 15Δ-PGJ2, DEHP, MEHP or MEOHP, respectively and the above described procedure was conducted. Each experiment was carried out in triplicate. The peptide identification was performed by the Protein Lynx Global Server 3.0.2 (Waters Corporation) and the deuteration level of each identified peptide was determined by DynamX 3.0 (Waters Corporation). Furthermore a biological assay (GeneBLAzer PPARγ, Invitrogen) was performed [3] to proof if the binding results in the biological activity of PPARγ.

The obtained HDX data showed significant shielding effects within the binding pocket of the PPARγ after treatment with the positive control 15Δ-PGJ2 and the phthalate metabolites MEHP and MEOHP. Thereby MEHP and MEOHP led to the typical activation associated conformational changes of the PPARγ that occur due to the binding of its endogenous ligand 15Δ-PGJ2 [4]. The most significant shielding effects could be observed in the α-helical regions H1-H2, H3-H4 and H7. These regions are known to be involved in the formation of the binding pocket within the ligand binding domain of the PPARγ [5]. Thus, it can be assumed that the DEHP-metabolites MEHP and MEOHP bind to the ligand binding pocket of the PPARγ while the phthalate DEHP itself showed no significant shielding effects and therefore no binding to the PPARγ. Furthermore, the biological assay confirmed that treatment with MEHP and MEOHP activates the PPARγ with EC10 values in the micromole range (1.2 µM and 0.45 µM, respectively).

In summary, this study provides the first molecular insights into the direct interaction of PPARγ with DEHP or its metabolites, respectively. It could be shown that there is an impact of one of the most frequently used phthalates DEHP on the PPARγ in vitro. However, not the DEHP itself binds and activates the PPARγ but its metabolites MEHP and MEOHP. Their role in the manifestation of the metabolic syndrome needs to be investigated by future studies in detail.

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Keywords – HDX-MS, PPARγ, phthalates, obesity

Analysis of serine-phosphorylation dependent protein-protein interactions of the T cell adaptor protein ADAP

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In T cell signaling reversible protein phosphorylation is an important feature, regulating many of the signal transduction pathways required for proper T cell functioning. The human adhesion and degranulation promoting adaptor protein (ADAP) plays a central role in T cell signaling [1]. Upon T cell receptor stimulation ADAP is strongly tyrosine-phosphorylated and serves as a hub for SH2 domain-containing effector proteins, which is a crucial event in signal transmission to integrins. Besides from this, several serine and threonine phosphorylation sites within the N-terminal domain of ADAP are phosphorylated. However, the role of these phosphorylation events in T cell signaling events has not been investigated.

Experimenteller Teil

LC-MS/MS measurements were performed using a capillary LC system (Dionex Ultimate 3000 NCS-3500 RS Nano, Thermo Scientific) connected to an Orbitrap Fusion or Elite mass spectrometer (Thermo Fisher Scientific). To identify new ADAP phosphorylation sites on serine residues in a complex matrix the dynamic range of the Orbitrap analyzer was extended by using a multiplexed TSIM method in combination with a data depend targeted HCD MS2 measurements using the ion trap as detector. For the identification of phosphorylation-dependent interaction partners of ADAP we use quantitative SILAC-based peptide and protein-pulldown approaches.

Ergebnisse und Diskussion

We demonstrate for the first time that two distinct phosphorylated serine residues in the N-terminal region of ADAP bind specifically to 14-3-3 isomers. Both ADAP-peptides containing either phosphorylated serine 155 or phosphorylated serine 235 show a phosphorylation dependent interaction with 14-3-3 isomers. The direct interaction of *in-vitro* phosphorylated ADAP and 14-3-3-zeta was validated by GST pulldown. The phosphorylation of serine 235 of ADAP was confirmed by the new developed TSIM method, where only precursor ions with a selected m/z are isolated and measured in the Orbitrap analyzer. Since 14-3-3 proteins are known for playing an important role in T cell signaling, this new phosphorylation dependent interaction between ADAP and 14-3-3-proteins may yield new insights into T cell signaling pathways [2], [3].

Neue Aspekte

Role of serine phosphorylation of the adapter protein ADAP in T cell signaling.

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Combining 2D-LC-MS and Gelfree-LC-MS enhances both proteome coverage and the identification of short open reading frame encoded peptides

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Archaea represent the second domain of Prokarya and despite their close physical resemblance to bacteria, they are phyolgenetically more closely related to eukarya. In the model archeaeon *Methanosarcina mazei*, carbon and energy metabolism have been well characterized, and the recent discovery of a number of small open reading frames (sORF) creates the need for suitable analytical technologies for the comprehensive identification of the corresponding gene products. For biological and functional studies the knowledge of the entire set of proteins and sORF gene products is essential. Consequently in the present study we evaluated analytical approaches that will allow for simultaneous analysis of widest parts of the proteome together with the predicted sORF.

Experimenteller Teil

We have utilized a combination of 2D-LC (high pH revered phase chromatographic fractionation followed by low pH ion pair reversed phase chromatography) and Gelfree-LC (GELFREE separation followed offline by low pH ion pair reversed phase chromatography) approaches, coupled to tandem MS analysis on a Thermo Q-Exactive plus mass spectrometer.

Ergebnisse und Diskussion

We performed a full proteome analysis of the methane producing archaeon *Methanosarcina mazei* strain Gö1 cytosolic proteome using a high/low pH reversed phase LC-MS bottom-up approach. The second analytical approach was based on semi-top-down strategy, encompassing a separation at intact protein level using a GelFree system, followed by digestion and LC-MS analysis. A high overlap in identified proteins was found for both approaches yielding the most comprehensive coverage of the cytosolic proteome of this organism achieved so far. The application of the second approach in combination with an adjustment of the search criteria for database searches further led to a significant increase of sORF peptide identifications, finally allowing to detect and identify 28 sORF gene products.

Neue Aspekte

The identification of sORF encoded proteins using modified proteome wide analytical methodologies.

Improved protocol for recovery of vesicular proteins

Sofia Traikov, Nikolaj Zuleger, Henrik Thomas, Anna Shevchenko, Andrej Shevchenko

Objective

Membrane-associated proteins are low abundant, yet biologically components of cellular organelles. Because of their poor solubility in commonly used buffers, they are difficult to identify by proteomics. We applied a lysis buffer with optimized composition, differential ultra-centrifugation and quantitative GeLC-MS/MS to dissect the composition of early endosome (EE) proteome from mouse liver. We demonstrate that having a millimolar concentration of magnesium chloride in a lysis buffer is a key for the high recovery of endosomal proteins.

Methods

Mouse liver was perfused and homogenized using sucrose-containing buffers with EDTA or $MgCl_2$. Early endosomes were purified using differential centrifugation in discontinuous sucrose gradients and the proteins were recovered by boiling in Laemmli buffer. Remaining membranes were pelleted and prepared in the same way as the endosomal fraction. Recovered EE-associated proteins and the proteins from the control membrane fraction were subsequently identified in GeLC-MS/MS experiments using a 3 h HPLC gradient for the analysis of each individual gel slab, and were then label-free quantified.

Results

Perfused mouse liver was homogenized using different sucrose-containing buffers in which their usual component (EDTA) was replaced with $MgCl_2$. After tissue homogenization, early endosomes were purified using differential centrifugation in discontinuous sucrose gradients and proteins were recovered by boiling in Laemmli buffer. Remaining membranes were pelleted and prepared in the same way as the endosomal fraction. The total membrane fraction was used as a control. Recovered EE-associated proteins and the proteins from the control membrane fraction were

quantified by label-free GeLC-MS/MS. In $MgCl_2$-containing preparations of EE vesicles, typical endosomal protein markers Rab5, Rab7, Lamp1/2 and AP-2, EGFR, Stabilin-1 and integrin were several folds enriched compared to the control. In total, we identified over 1,500 proteins in combined EE fractions and additionally 250 proteins, inlcluding effector EEA1 or members of the ESCRT machinery, transmembrane proteins (Sortilin) or adaptors (AP3 delta) along with 30 new proteins whose biological relevance is now being evaluated, were only detectable in extracts with $MgCl_2$.

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Novel aspect

$MgCl_2$ dramatically increases the recovery of EE-proteins.

Quantitative proteomics for the analysis of molecular changes in lung adenocarcinoma cells in response to Vitamin D_3

Patrick Kaleja[1,2], Liam Cassidy[1], Sabine Fuchs[2], Andreas Tholey[1]

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Keywords: Quantitative Proteomics, 2D-LC MS, Isobaric Labeling, Alveolo-Capillary Barrier

The alveolo-capillary barrier in human lungs fulfils essential functions, e.g. gas exchange and defence against pathogens. Pathological processes in the lung, such as infection and inflammation, may lead to loss of barrier integrity and thus result in dramatic effects for patients. Supplementation of Vitamin D_3 (VD3) has been shown to have a significant, strengthening effect on the alveolar barrier in a lung adenocarcinoma model and can compensate integrity loss in the presence of lipopolysaccharides.
Since only single proteins are known to respond to VD3 treatment in alveolar cells, we aimed to expand characterization of this model to a proteome wide level. A quantitative proteomics approach was used analysing individual protein abundance changes after supplementing our cell model with VD3.
Besides analysing the effect of VD3 on the barrier function of lung adenocarcinoma cells H441 on cellular level via molecular biological experiments, three biological replicates of treated and untreated cells were lysed for quantitative isobaric TMT-sixplex bottom-up proteomics study. Following methanol-chloroform precipitation, reduced and alkylated protein lysates of each replicate were tryptically digested and labelled with one corresponding TMT-reagent. Applying two dimensional, semi-orthogonal chromatography via high pH/ low pH eluents on reversed phase columns, pooled peptide fractions were measured online on a Q Exactive Orbitrap mass spectrometer in four technical replicates by $ddMS^2$. Data analysis was performed via Thermo Proteome Discoverer and TMT-ratios were corrected on the basis of peptide interference level.
We identified more than 7,200 proteins of which 6,455 proteins were quantified; 56 proteins displayed a significant abundance change induced by treatment with VD3. The identified molecules ranged from constitutional extracellular matrix components, surfactant associated-, to immune-regulatory molecules. While some previously in the literature described VD3 associated proteins were verified, other proteins yet not linked to VD3 treatment could be identified, providing a wider insight into the different pathways related to this micronutrition. Furthermore, these newly identified proteins enable targeted analysis and may lead to new therapeutic strategies for patients in the future.

New aspects: Identification of cellular adaptation to VD3 in an alveolo-capillary barrier *in vitro* model via quantitative proteomics.

Title: Limit 20 words

Accelerating Data Independent Acquisition with Microflow Chromatography

Joerg Dojahn[1], Nick Morrice[2], Remco Van Soest[3], Christie L Hunter[3]

[1]SCIEX, Germany; [2]SCIEX, UK; [3]SCIEX, Redwood City, CA

Introduction:

Data independent acquisition (DIA) strategies have been used to increase the comprehensiveness of data collection while maintaining high quantitative reproducibility. Many labs are now using DIA to perform larger scale quantitative proteomic experiments with solid reproducibility on 1000s of proteins in complex matrices. As this technique increasingly proves to be a solid tool for biomarker research, larger sample sets are being analyzed, driving the need for further investigation of workflow improvements for throughput and robustness. Here microflow LC with 15cm columns and 45-60min gradients was investigated in combination with SWATH® acquisition, to assess depth of coverage and robustness relative to current nanoflow strategies. In addition we describe the improvements in protein quantitation coverage with SWATH® acquisition using longer µLC columns and gradients.

Methods:

Separation of a trypsinated HEK cell lysate was performed on a NanoLC™ 425 System (SCIEX) operating in microflow mode using a single 15 cm x 0.3 mm ID 3 µm C18 column, and a 30 cm long column by coupling two columns together. Gradients of 45 and 90 minutes where used. Total protein injected on column ranged from 1 – 8 µg. The MS analysis was performed on a TripleTOF® 6600 system (SCIEX). Variable window SWATH® Acquisition methods were built using Analyst® TF Software 1.7. Replicate injections of each acquisition condition were processed using SWATH® 2.0 Software. All protein and peptide numbers reported were determined at <1%FDR and <20% CV across the 5 replicates collected.

Results and discussion:

Higher sample loads up to 8µg and increasing numbers of variable sized Q1 windows provided progressively more quantified peptides and proteins. Under the final conditions, ~5000 proteins can be quantified from a cell lysate protein in a 1 hour time frame. In comparison to previous nanoflow results, we achieved ~85% of the quantified proteins but with ~400% higher throughput.

Increasing column length to 30 cm and using the same gradient showed only a minimal improvement. When combining the use of a longer column with the 100 min gradient, increased numbers of quantifiable peptides/proteins were seen (27%, 17%).

When more sample is available to move to the higher flow rate regime, very high reproducibility is achievable with faster run times.

Novel aspect: 20 words

Accelerating SWATH acquisition (DIA) with microflow LC to industrialize quantitative proteomics

Evaluation of Optimal Conditions for Antibody Subunit Analysis on a Quadrupole-Orbitrap Mass Spectrometer

Kai Scheffler, Tabiwang Arrey, Martin Zeller and Eugen Damoc

Introduction

MS analysis of antibodies at the protein and peptide levels is critical during development and production of biopharmaceuticals. The compositions of current generation therapeutic proteins are often complex due to various modifications which may affect efficacy. Intact mass and peptide mapping analyses have become essential techniques in mAb analysis. The analysis of antibody subunits often provides additional and complementary information with the advantage of requiring only very little sample preparation. Reduction is an optional step in the sample preparation, and when combined with enzymatic digestion with IdeS resulting in ~23-25 kDa subunits. Subunits in that molecular weight range are most amenable to top-down analysis and can provide highest sequence coverage.

Experimental

Here we have reviewed three commercially available monoclonal antibodies under different reduction conditions aiming at complete reduction of inter- and intra-chain disulfide bridges and most efficient fragmentation and sequence coverage in top-down experiments.
The mass spectrometer used for all experiments was a commercially available hybrid quadrupole-Orbitrap mass spectrometer equipped with the new BioPharma option.

Results and discussion

For top-down analysis the presence of disulfide bridges is a generally limiting factor preventing efficient fragmentation in particular in the regions between two cysteine residues involved in a disulfide bridge. Whereas the reduction of inter-chain disulfide bridges is often very efficient, reduction of the intra-chain disulfide bridges often require more stringent conditions for efficient reduction and show higher variability amongst different antibodies.

We discuss results obtained for different reduction conditions as well as optimized chromatography and mass spectrometry conditions and parameter settings as well as method options for optimized antibody subunit characterization.

Novel aspect

Method optimization for antibody disulfide bridge reduction prior to top-down characterization

Characterization of plastidal redox-responses during cold stress acclimation.

Johannes Schütze[1], Stephanie Doell[1,2], Hans-Peter Mock[1]

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Introduction

Organisms are able to adapt to many different environmental changes, due to alteration in der protein content. The cold stress response of the *Arabidopsis thaliana* has been performed analysing charges on the transcriptional level. However, proteomic studies on cold stress response of plants are still limited. Here we analysed the whole leaf proteome of *Arabidopsis* plants exposed to low temperature for one week. Results indicated a strong response of the plastidal proteome. As a second part of our study we hence aim at detailed proteome analysis of isolated plastids.

Experimental section

Five week old wild type *Arabidopsis thaliana* were harvested after one week of cold stress conditions (10°C for 1 week, 20°C control). The leaf proteins were extracted, tryptically digested and the resulting peptides separated with LC-MS.

For the plastidal experiments the cell compartments were separated by different centrifugation steps. Purified chloroplasts were further separated into a stromal fraction containing soluble proteins and a thylakoid fraction. Proteins were and all samples were digested using a in filter digestion method and the resulting peptides were separated using LC-MS. extracted by liquid extraction and salt assisted protein extraction. All samples were digested using an in filter digestion method.

Results and discussion

We were able to identify around 800 proteins with at least one unique peptide. 110 of the proteins were significantly more abundant in 10°C treated plants and 88 more abundant in 20°C. The regulated proteins could be sorted into different groups according to their biological functions. 64 proteins are related to different metabolic processes. 37 proteins are more abundant in regulation processes for 10°C and 7 are higher abundant in 20°C. The category “response to stimulus” contents 29 proteins for 10°C and 9 for 20°C. The other proteins were be assigned to other categories, such as “Cellular organization” “Cell redox homeostasis” and “Localization. The analysis of the leaf proteome of *Arabidopsis thaliana* provided valuable informations about the cold stress acclimation of plants in general.

Based on the results of the whole proteome analysis, we initiated a detailed study of the plastidal proteome. After optimizing the isolation of plastids from cold-treated plants, we are currently performing the LC-MS analysis of the isolated plastidal proteome fractions.

Novel Aspects

Cold stress responses of the *Arabidopsis* leaf and plastidal proteome.

Keywords

Proteomics, Cold stress, Plastids, *Arabidopsis thaliana*

Innovative analytical methodologies for the development of new antitubercular agents

Francesca Rinaldi[1], Sara Tengattini[1], Caterina Temporini[1], Enrica Calleri[1], Gabriella Massolini[1], Loredana Lupu[2,3], Zdeněk Kukačka[2], Stefan Maeser[2], Michael Glocker[3], Michael Przybylski[2]

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Introduction

Tuberculosis (TB) is an infectious disease caused by *Mycobacterium tuberculosis* (*Mtb*) and it still constitutes a considerable threat for human health [1]. A strategy to fight TB could be the design of a glycoconjugate vaccine composed of carbohydrate moieties coupled to an immunogenic carrier molecule able to induce both humoral and T cell-mediated immune responses, resulting in an improved antigenicity compared to the single constituents [2]. Ag85B was selected as a carrier protein since it is one of the most potent antigen species expressed by *Mycobacterium tuberculosis* (*Mtb*) yet identified [3]. The protein was conjugated with simple saccharidic moieties activated with the iminomethoxyethyl functional group [4], which selectively reacts with the ε-amino group of lysine residues [2].

Experimenteller Teil

Experimental section

The immunogenic protein and its glyco-conjugates were deeply characterized.

MALDI-MS analyses of the samples were performed using an autoflex III smartbeam mass spectrometer (Bruker Daltonik, Bremen, Germany). Moreover, two enzymatic digestions of Ag85B protein were performed in parallel using trypsin and chymotrypsin and analyzed by MALDI-MS.

Affinity binding experiment were carried out on a SR7500DC (Reichert, Depew, NY) instrument. The *Mycobacterium tuberculosis* Ag85 antibody was immobilized on a SPR carboxymethil dextran chip and dilution series from 0.2 to 6.4 µM of Ag85B and some mutant forms of this protein were analyzed.

Ergebnisse und Diskussion

Results and discussion

One of the main problems in vaccine development is the lack of a clear correlation between design and protection [5]. For this reason, the pharmaceutical analysis played a crucial role at all the stages of the research.

At first, MALDI-MS analyses of the intact protein and its glycosylated forms were performed to define identity and purity of the samples and to assess the glycosylation profile. In addition, a peptide mapping was carried out on Ag85B, which was enzymatically digested with trypsin and chymotrypsin. Intact mass measurements confirmed the identity and purity of Ag85B

recombinant protein and proved the effectiveness of the glycosylation procedure, which resulted in the production of different glycoforms. The peptide mapping allowed to verify the protein sequence, resulting in a good coverage for both the enzymatic digestions.

Furthermore, SPR technology was employed to determine vaccine affinity for IgG antibodies. *Mycobacterium tuberculosis* Ag85 antibody was selected as a model to study the interaction. The affinity was investigated comparing the wild type protein with some mutants designed to prevent the glycosylation reaction towards antigenic amino acids and to improve the immunogenicity of the glycoconjugates. Analyses allowed to obtain a dissociation constant in the nanomolar range for Ag85B and to highlight that wild type protein binds to the antibody more strongly than its mutants.

Neue Aspekte

Novel aspects

Different analytical techniques were exploited to characterize a potential vaccine against TB and to improve its rational design.

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Sampling of tissues with the picosecond-infrared-laser ablation for Redox Proteomics

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Introduction

Post-translational modifications induced by oxidation reactions (Ox-PTMs) are associated with regulation of different cellular functions as well as diseases [(1, 2)]. Therefore, advances in the analysis of Ox-PTMs of proteomes including methionine oxidation will provide a better understanding of disease mechanisms including cancer. We present a novel, soft technology for cold vaporization of tissues through desorption by impulsive vibrational excitation (DIVE) of intramolecular vibrational states of intracellular water molecules by irradiating the samples with a picosecond-infrared-laser (PIRL) [(3, 4)]. In this study we compared the degree of oxidation of methionine containing peptides of tissue homogenates yielded either by PIRL or classical homogenization.

Key words, picosecond-infrared-laser, methionine oxidation, cancer, LC-MS/MS

Experimental Section

Rat pancreas tissue was cut into 2 equal pieces and frozen. The tissue samples were homogenized in Laemmli buffer either mechanically using a bead mill (TissueLyser II) or by cold vaporization via laser ablation with PIRL-DIVE.

The ablation plume was collected in a falcon tube (cold trap) placed in liquid nitrogen. The samples were in-gel digested. The tryptic peptides were analyzed using LC-MS/MS. LC–MS/MS measurements were performed by injecting the samples on a nano liquid chromatography system (nanoACQUITY, Waters, Manchester, UK) coupled via (ESI) to a quadrupole orbitrap mass spectrometer (Orbitrap QExcactive, Thermo, Bremen, Germany).

The identification and quantification of methionine containing peptides was performed by processing mass spectrometric data using MaxQuant, searching against Rattus norvegicus database.

Results and discussion

Equal pieces of pancreas tissues were used for PIRL-DIVE and for mechanical homogenization. In the PIRL-DIVE prepared sample 1533 methionine-containing peptides were detected. 1388 of these were detected both in the oxidized and in the reduced form, allowing the determination of the degree of oxidation for each peptide. In the sample obtained by mechanical homogenization the total number of identified methionine-containing peptides was 2382 with 1238 peptides detected both in the oxidized and in the reduced state.

In the PIRL-DIVE homogenized samples 54 methionine containing peptides (3.9%) were detected, in which larger relative amounts of oxidized species than reduced species (ratio oxidized/reduced >1) were detected, while in the case of 1334 methionine-containing peptides (96.1 %) the ratio oxidized/reduced was < 1.

In contrast in the mechanically homogenized samples in the case of 50% of the methionine-containing peptides the oxidized species were present in higher amounts than the reduced species (ratio oxidized/reduced >1). In the group of the other 50% the oxidized species was present in lower amounts than the reduced species (ratio oxidized/reduced < 1).

The percentage of oxidized methionine containing peptides to the total number of identified peptides was 7.25% in PIRL compared to 16.40% in mechanical homogenization.

Our results demonstrate, that during PIRL-DIVE homogenization less oxidation occurs. Therefore it is better suited for investigation of the physiologic redox state of proteomes than classical homogenization procedures.

New aspect

PIRL-DIVE, newly introduced, can serve as a new, ultrafast method in the investigation of redox proteome in the cell.

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Partial Immunoblotting of 2D-Gels: A Novel Method to Identify Post-Translationally Modified Proteins Exemplified for the Myelin Acetylome

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Introduction. Post-translational modifications (PTMs) play a key role in regulating protein function, yet their identification is technically demanding. Particularly for oligodendrocytes, a glial cell type forming the myelin sheath in the central nervous system, information on PTMs is limited. 2D immunoblotting is predestined to be used for targeted PTM screening when specific antibodies are available as is the case for lysine acetylation. However, the major challenge of this approach is the correct matching of the two 2D-gels that are typically run in parallel, one for blotting and immunodetection, and the other for protein staining, excision of spots of interest, and mass spectrometric protein identification. Here, we present a straightforward 2D immunoblotting method for reliable multiplexing of PTM screening and protein identification.

Experimental section. Myelin proteins are separated by 2D gel electrophoresis (2DE), stained with colloidal Coomassie, and the stained proteins are then partially transferred onto a PVDF membrane that can be subjected to immunodetection with PTM-specific antibodies. As a fraction of each protein is retained in the original gel, immunopositive proteins can be tracked back and mass spectrometrically identified from the same protein spot, thereby avoiding false assignment to abundant proteins migrating nearby. Subsequent validation of the protein identified can be readily included by its immunodetection in a second detection channel using the same PVDF membrane. Signals are consistently detected by near-infrared fluorescence imaging at all levels.

Results and discussion. We exemplify the power of partial immunoblotting with the identification of lysine-acetylated proteins in myelin, the oligodendroglial membrane that insulates neuronal axons (Jahn et al., *Mol. Neurobiol.* 2009, 40:55-72). Transferred myelin proteins were detected by staining with colloidal Coomassie and by immunodetection with antibodies directed against acetylated lysine (AcK). Image overlay revealed 20 AcK-positive spots, from which 11 potentially acetylated proteins were identified. For most of these myelin proteins, lysine acetylation was already described in other tissues. The strongest AcK signal was obtained from spots containing α- and β-tubulin proteins, which was validated by using a second primary antibody specific for α-tubulin. As acetylation at K^{40} of α-tubulin is known to mediate microtubule stabilization in axons, the long projections of neuronal cells (Yu et al., *J. Biol. Chem.* 2015, 290:17163-17172), we used immuno-electron-microscopy of optic nerves to rule out that acetylated α-tubulin was detected in the myelin fraction only due to axonal contamination. As expected, AcK^{40}-α-tubulin was highly abundant in axons, but absent in compact myelin. Interestingly, the adaxonal and abaxonal non-compact myelin compartment containing cytosol with microtubules were positive for AcK^{40}-α-tubulin. To show acetylation of α-tubulin at K^{40} in the myelin fraction, 2D gel spots that were found to be highly immunopositive for AcK and to contain α-tubulin were excised and subjected to in gel digestion with endoproteinase AspN. Mass spectrometric peptide sequencing of AcK^{40}-α-tubulin(39–68) by MALDI-TOF-MS/MS and electrospray LC-MS/MS confirmed the identity of the tubulin peptide AcK^{40}-α-tubulin(39–68). In conclusion, our multi-level workflow holds great promise for the identification of PTMs for which specific antibodies are available, and can be readily adapted to clinical applications such as identifying auto-immune antigens or host-pathogen interactions.

Novel aspects. A 2DE-based low-tech method for comparative PTM screening that is easily adaptable to any kind of antibody-detectable protein modification.

Keywords. Post-translational modification, 2D gel electrophoresis, myelin, acetylome, tubulin acetylation

Mass Spectrometric Characterization of Proteins from condensates of the Picosecond Infrared Laser Ablation

Marcel Kwiatkowski[1,2]

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Protein species are defined as the smallest unit of the proteome. The function of a protein species depends on its exact chemical composition. Even small changes in its composition can change its function. For investigation of molecular mechanisms in cells at the protein level it is therefore important to detect protein species in their *in-vivo* state.

Experimenteller Teil

During protein extraction from tissues there is a risk that the chemical compositions of protein species is changed by both enzymatic and chemical reactions. Cold tissue vaporization by the picosecond infrared laser (PIRL) represents a soft procedure for tissue ablation originally developed for medical laser surgery [1]

Ergebnisse und Diskussion

It was hypothesized that PIRL ablation represents a new and innovative method for releasing intact protein species from tissue samples without changing their chemical composition. This assumption was confirmed by different mass spectrometry methods and differential proteomics. It has been shown that the chemical composition of RNase A as well as the chemical composition of the phosphoproteins alpha-S1-, alpha-S2- and beta-casein was not changed by PIRL ablation. In addition, trypsin as well as proteases in human blood plasma were still enzymatically active after PIRL ablation, which indicates that proteins are not significantly denatured during PIRL ablation [2]. Differential analysis of protein extracts from human tonsils generated either by PIRL ablation or by conventional methods revealed a significantly lower number of proteolysis products and a considerably higher number of protein species in case of PIRL ablation [3]. From these results, it was concluded that the PIRL ablation enables a better access to the original protein species composition of tissues. Due to the ultrafast and soft tissue vaporization, intact protein species are exposed to a significantly lesser extend to enzymatic degradation reactions through proteases and other enzymes. The explosive but gentle transformation of tissues into aerosols presumably is the reason for the generation of homogenates, which are almost free of particles and therefore responsible for the high yield of identified protein species. Therefore, the PIRL ablation should in the future make the study of tissue proteomes at the protein species level more reliable with respect to their original *in-vivo* composition.

Neue Aspekte

Ps MALDI Ablation

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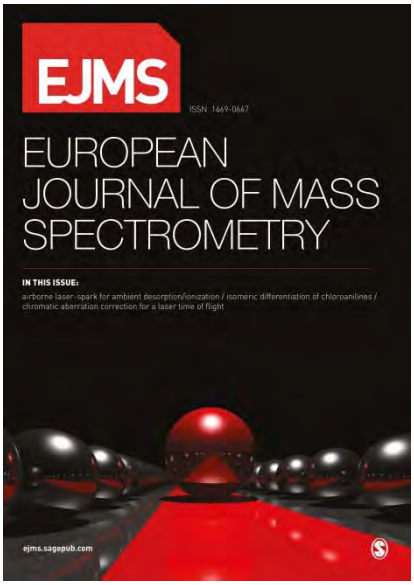

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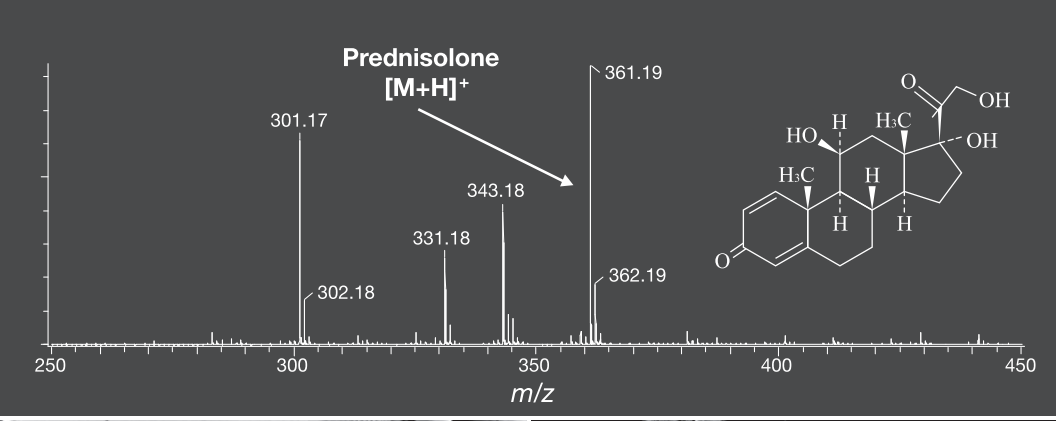

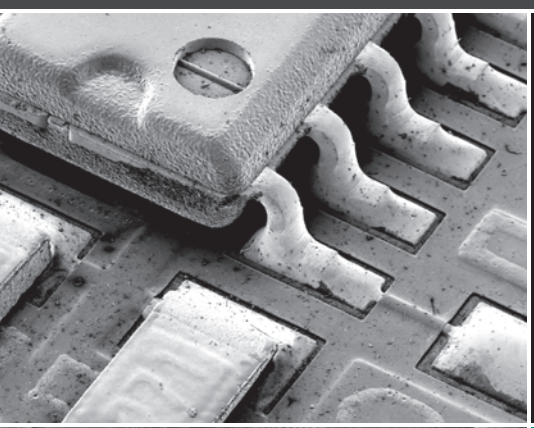

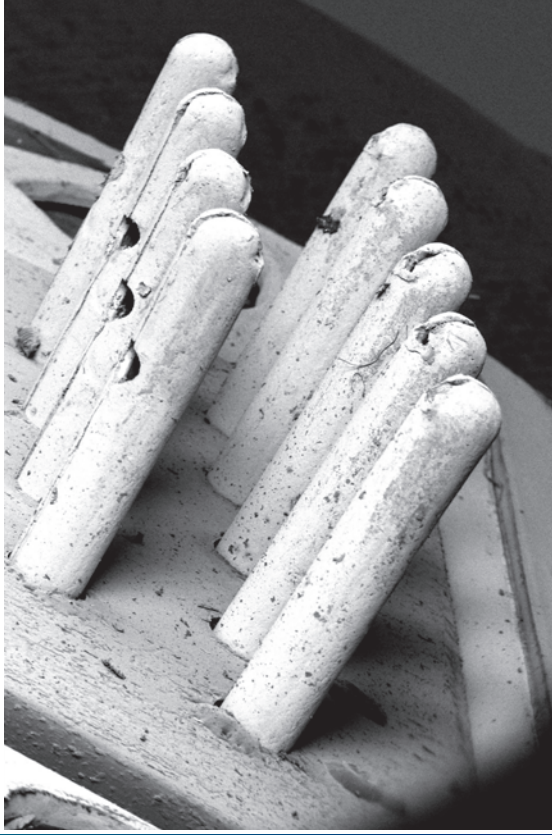

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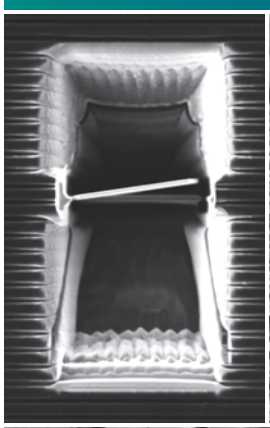

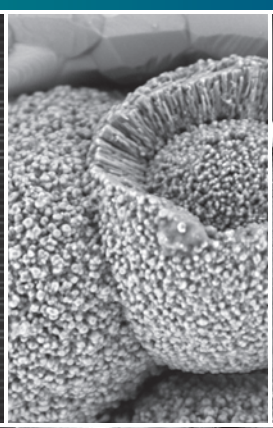

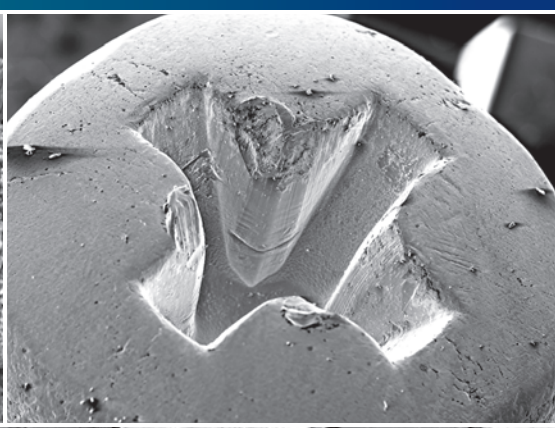

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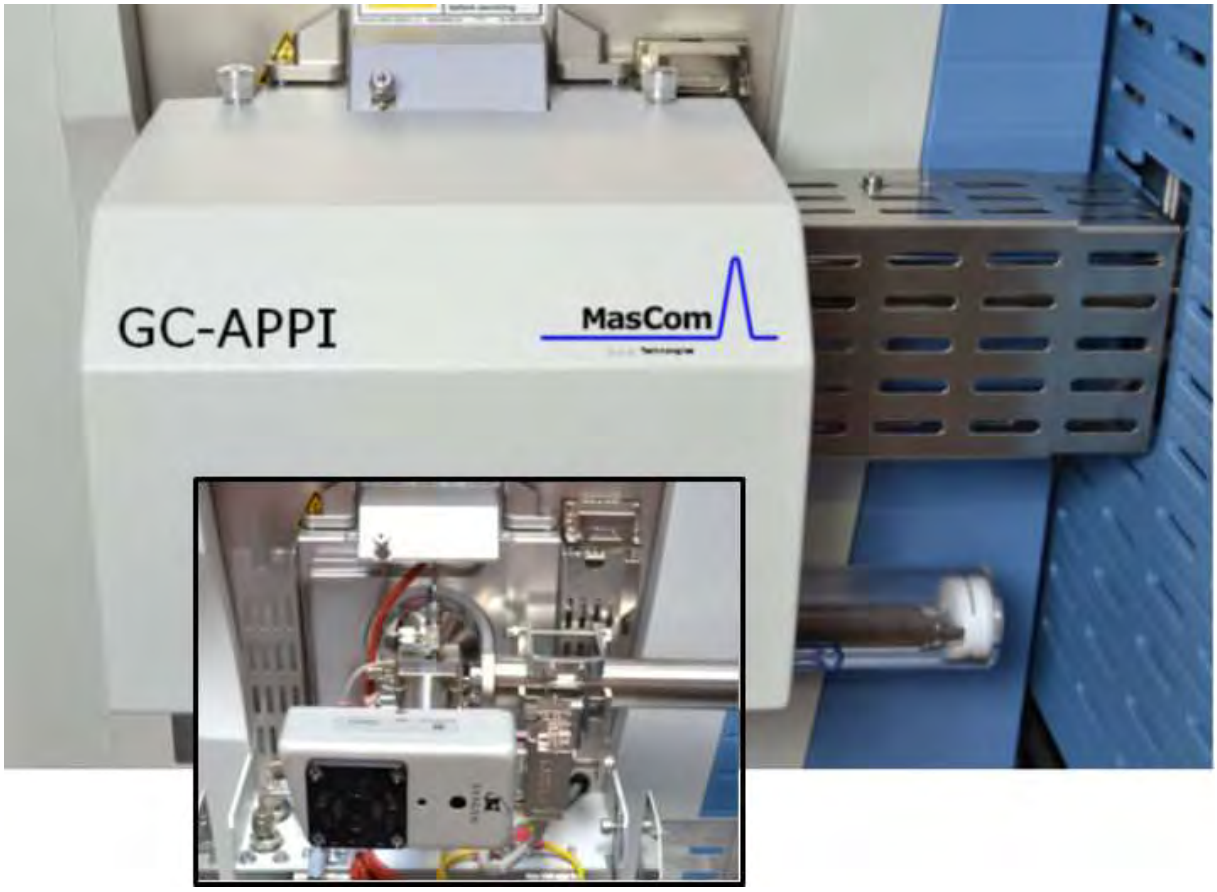

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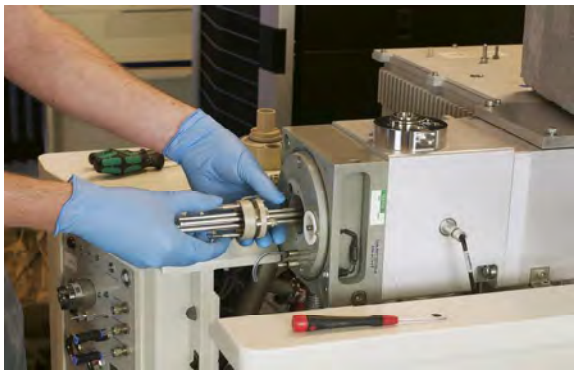

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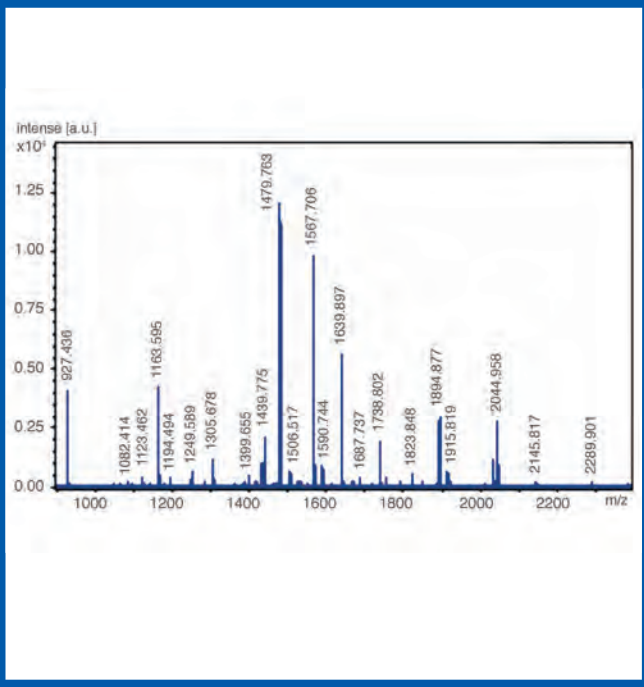

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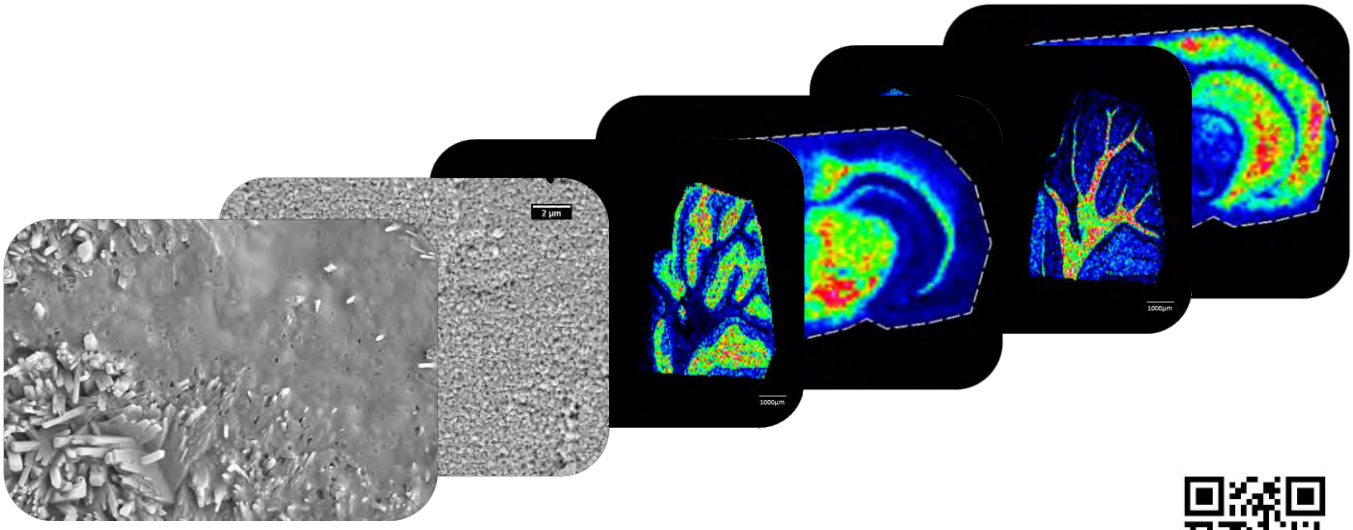

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