All orals will be a part of the on-demand content for the ASMS 2020 Reboot. Registrants will have access to the short abstract, ePoster, and optional poster presentation video June 1 - August 31, 2020 via the mobile app and online planner (these tools become available on June 1.)

In addition there will be a webinar ‘Watch party’ followed by Live Q&A with speakers in week 2 of the Reboot program (June 8-12). ‘Watch party’ will be viewing of the six talks (also available on-demand at any time beginning June 1.) Registered attendees interested in only the Live Q&A will be advised to join the webinar after approximately two hours (time for six 20-minute talks to play.)

Note that some sessions have 'empty slots' listed. For these sessions chairs will seek to find alternates from among the poster presenters. We will update this Orals document as alternates for these slots are confirmed.

Thank you for your interest in the ASMS 2020 Reboot program. More information on the Reboot may be found here. To register and have the full-access described above, please go here.

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WEDNESDAY PM ORALS ........................................................................................Page 24
THURSDAY AM ORALS........................................................................................Page 29
THURSDAY PM ORALS........................................................................................Page 33
MONDAY AM ORALS

MOA am: Instrumentation: Innovations in Mass Analyzers
Chair: Chad Weisbrod (National High Magnetic Field Laboratory)

MOA am 08:30 Coulombic interaction as a new ion ejection method for ion trap mass spectrometry analysis; Xiaoyu Zhou1; Zheng Ouyang1; 1Tsinghua University, Beijing, China

MOA am 08:50 Microparticle charge detection mass spectrometry using printed circuit board arrays; Eflaura Gustafson1; Tabitha Caldwell1; Daniel E. Austin1; 1Brigham Young University, Provo, UT

MOA am 09:10 Highly Multiplexed Individual Ion Mass Spectrometry in an Orbitrap for Both Native and Top-Down MS; Jared O. Kafader1; Ping F. Yip2; Bryan P Early1; Kenneth R Durbin1; Neil L. Kelleher1; Michael W. Senko2; Philip D. Compton1; 1Northwestern University, Evanston, IL; 60208; 2Thermo Fisher Scientific, San Jose, CA

MOA am 09:30 Parallel DDA and DIA acquisition of spectra in an ion cyclotron resonance array cell; Jared P. Mohr1; Sung-gun Park1; Gordon A. Anderson2; James E. Bruce3; 1University of Washington, Seattle, WA; 2GAA Custom Engineering, LLC., Benton, WA

MOA am 09:50 FT mass spectrometer based on multielectrode harmonized Kingdon trap in FT ICR mode of operation; Eugene (evgeny) Nikolaev1,2; Oleg Kharybin3; Gleb Vladimirov1; 1Skolkovo institute of science and technology, Moscow Region, Russian Federation; 2Institute of Energy Problems of Chemical Physics Russian Academy of Sc., Moscow, Russia; 3Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation

MOA am 10:10 A novel compact Orbitrap platform enables new applications of high-resolution accurate-mass analysis; Jan-Peter Hauschild1; Amelia Peterson1; Erik Couzijn1; Eduard Denisov1; Denis Chernyshev1; Christian Thoeing1; Oliver Lange1; Bastian Reitemeier1; Arne Kreutzmman1; Wilko Balschun1; Aivaras Venokus1; Sebastian Kanngiesser1; Alexander Kholomeev1; Gregor Quiiring1; Frank Czemper1; Kerstin Strupat1; Siegrun Mohring1; Tabiwang N. Arrey1; Julia Kraegenbring1; Catharina Crone1; Mathias Mueller1; Andreas Wieghaus1; Alexander Makarov1; 1Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

MOB am: Ion Mobility: Structure
Chair: Tara Pukula (University of Adelaide)

MOB am 08:30 Ion mobility spectra of fragment ions produced from native top-down sequence analysis reflect type and sequence of the fragment ions; Christian Bleiholder1; Fanny C Liu1; Kirsten Tucker1; 1Florida State University, Tallahassee, FL

MOB am 08:50 Annotating Collision Induced Unfolding Pathways using Electron Capture Dissociation; Carolina Rojas Ramirez1; Ruwan T. Kurulugama2; Valery G. Voinov2; John C. Fjeldsted2; Brandon T. Ruotolo2; 1University of Michigan, Ann Arbor, MI; 2Agilent Technologies, Santa Clara, CA; 3-e-MSion, Inc., Corvallis, OR

MOB am 09:10 Use of Ion Mobility-Mass Spectrometry (IM-MS) to Characterise the Structures of Poly(L-Lysine) Dendrimers; Florian Benoit1; Richard M. England1; Tony W. T. Bristow1; 1Manchester Institute of Biotechnology, Manchester, United Kingdom; 2AstraZeneca, Macclesfield, United Kingdom

MOB am 09:30 FAIMS and native mass spectrometry: Analysis of intact protein assemblies and protein complexes; Oliver J Hale1; Eva Illes-Toth1; Todd H. Mize1; Helen Cooper1; 1University of Birmingham, Birmingham, United Kingdom

MOB am 09:50 High-Resolution Ion Mobility Separations of Isomeric Glycoforms with Variations on the Peptide and Glycan Levels; Pratima Pathak1; Matthew A. Baird1; Alexandre A. Shvartsburg1; 1Wichita State University, Wichita, KS

MOB am 10:10 Are the structures of molecular elephants enduring or ephemeral? Results from time-dependent, tandem ion mobility; Benjamin P Zercher1; Seoyeong Hong1; Anneclaire Wageman1; Matthew Bush1; 1University of Washington, Seattle, WA
<table>
<thead>
<tr>
<th>Time</th>
<th>Title</th>
<th>Authors</th>
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<tr>
<td>MOD am 08:30</td>
<td>The many and varied responses of different varieties and species of rice to a range of external stresses; Sara Hamzelou; Fatemeh Habibpourmehraban; Matthew McKay; Aradesh Amirkhani; Karthik Kamath; Mehdi Mirzaei; Brian J. Atwell; Paul A. Haynes; Macquarie University, North Ryde, Sydney, Australia</td>
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<tr>
<td>MOD am 08:50</td>
<td>Development of data-independent acquisition (DIA) peptidomics approach on analyzing peptide signaling in plants; Yet-Ran Chen; Sheng-Chih Hung; Wei-Hung Chang; Ying-Lan Chen; Academia Sinica, Taipei, Taiwan; National Taiwan University, Taipei, Taiwan</td>
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<tr>
<td>MOD am 09:10</td>
<td>Identification of antimicrobial peptides from plants; Tessa B. Moyer; Lilian R. Heil; Leslie M. Hicks; UNC-Chapel Hill, Chapel Hill, NC</td>
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<tr>
<td>MOD am 09:30</td>
<td>Visualizing the distribution of strawberry plant metabolites at different maturity stages by MALDI imaging mass spectrometry; Jin Wang; Ethan Yang; Pierre Chaurand; Vijaya Raghavan; McGill University, Sainte-Anne-de-Bellevue, QC; University of Montreal, Montreal, QC</td>
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<tr>
<td>MOD am 09:50</td>
<td>Mass Spectrometry Elucidates Benzothiadiazole-Induced Immunity to a Bean Rust Fungus; Bret Cooper; USDA-ARS, Beltsville, MD</td>
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<td>MOD am 10:10</td>
<td>A draft of the Arabidopsis proteome; Julia Mergner; Martin Frejno; Markus List; Maxim Messerer; Daniel Lang; Xia Chen; Ajeet Chaudhary; Hiromasa Shikata; Philipp Cyprys; Rashmi Hazarika; Daniel Zolg; Patroklos Samaras; Tobias Schmidt; Mathias Wilhelm; Stefanie Sprunk; Jan Baumbach; Frank Johannes; Klaus Mayer; Kay Schneitz; Claus Schwechheimer; Bernhard Kuster; TU Munich, Freising, Germany; Helmholtz Center, Munich, Germany; Institute of Transformative Bio-Molecules, Nagoya, Japan; University of Regensburg, Regensburg, Germany</td>
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<tr>
<td>MOD am 08:30</td>
<td>MassIVE.quant: a community resource of curated quantitative mass spectrometry-based proteomics datasets; Meena Chai; Jeremy Carver; Cristina Chiva; Manuel Tzouros; Ting Huang; Tsung-Heng Tsai; Benjamin Pullman; Oliver M. Bernhardt; Ruth Hüttenthal; Guo Ci Teo; Maria Pavlou; Erik Verschueren; Bernd Wollscheid; Alexey I. Nesvizhskii; Lukas Reiter; Tom Dunkley; Eduard Sabido; Nuno Bandeira; Olga Vitek; Northeastern University, Boston, MA; University of California San Diego, San Diego, La Jolla, CA; Barcelona Institute of Science and Technology, Barcelona, Spain; Proteomics Unit, Center for Genomic Regulation, Universitat Pompeu Fabra, Barcelona, Spain; Roche Pharma Research and Early Development, Pharmaceutical Sciences, Roche Innovation Center Basel, Basel, Switzerland; University of California San Diego, San Diego, CA; Biognosys, Schlieren, Switzerland; University of California San Francisco, San Francisco, CA; University of Michigan, Ann Arbor, MI; Institute of Molecular Systems Biology, Zürich, Switzerland</td>
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<td>MOD am 08:50</td>
<td>Millisecond informatics: real-time analytics for quantitative proteomics; Devin K Schwepppe; Edward L Huttlin; Ramin Rad; Qing Yu; Jimmy K Eng; Jose Navarrete-Pereza; João A Paulo; Steven P Gygi; Harvard Medical School, Boston, MA; University of Washington, Seattle, WA</td>
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<td>MOD am 09:10</td>
<td>A Novel Method for Detection of Differential Alternative Splicing in MS Proteomics Data; Constantin Ammar; Gergely Csaba; Markus Gruber; Ralf Zimmer; Ludwig-Maximilians-Universität München, Munich, Germany</td>
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<td>MOD am 09:30</td>
<td>Deep neural network embedding for efficient repository-scale analysis of hundreds of millions of mass spectra; Wout Bittremieux; Damon May; Jeffery A. Bilmes; William Stafford Noble; UCSD, La Jolla, CA; University of Washington, Seattle, WA</td>
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<td>MOD am 09:50</td>
<td>Peptide grouping within protein coding genes: A proteofrom tolerant model for protein quantification in bottom-up proteomics; Deanna L Plubell; Kianna Hailes; Jea Park; Lukas Kall; Gennifer Merrithew; Thomas J. Montine; Michael J MacCoss; University of Washington, Seattle, WA; Royal Institute of Technology, Stockholm, Sweden; Stanford University, Palo Alto, CA</td>
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<td>MOD am 10:10</td>
<td>Extending Prosit to the prediction of proteotypicity, precursor ion charge and ion mobility collisional cross sections; Tobias Schmidt; Michael Graber; Siegfried Gesslat; Daniel P Zolg; Tobias Rohde; Brendan Maclean; Patroklos Samaras; Johannes Zerweck; Tobias Knaute; Bernard Delange; Andreas Huhmer; Karsten Schnatbaum; Ulf Reimer; Bernhard Kuster; Mathias Wilhelm; Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; University of Washington, Seattle, WA; JPT Peptide Technologies GmbH, Berlin, Germany; Thermo Fisher Scientific, Bremen, Germany; Thermo Fisher Scientific, San Jose, CA</td>
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Biomarkers in FFPE Tissues
A GCLP Quantitative Mass Spectrometry Workflow for Multiplexed Measurement of Protein Biomarkers in FFPE Tissues

MOE am: Microorganisms and the Microbiome
Chair: Vanessa Phelan (University of Colorado, Denver - Anschutz)

MOE am 08:30
Combatting fungal infections through the discovery and elucidation of novel anti-virulence strategies; Brianna Ball1; Duncan Carruthers-Lay2; Elizabeth Woroszchuk3; Jennifer Geddes-McAlister4; 1University of Guelph, GUELPH, ON

MOE am 08:50
Proteomics Reveal the Underlying Mechanisms of Filamentous Persisters during Ampicillin Treatment and Resuscitation; Jordy Evan Sulaiman1; Henry Lam1; 1The Hong Kong University of Science and Technology (HKUST), Clear Water Bay, Hong Kong

MOE am 09:10
Minimum Inhibitory Concentration Determined by Incorporation of Deuterium in Microbial Lipids; Matthew Sorensen1; Francesca Gardener2; David R Goodlett3 4; Robert K Ernst3; Erik Nilsson1; 1Pataigin, LLC, Baltimore, MD; 2University of Maryland, Baltimore, Baltimore, MD; 3University of Maryland, Baltimore, MD; 4International Centre for Cancer Vaccine Science, Gdsnsk, Poland

MOE am 09:30
Deciphering Host Immune Responses to Staphylococcus aureus Infection by Combining Imaging Mass Spectrometry and CODEX Multiplexed Immunofluorescence; Elizabeth Kathleen Neumann1 2; Nathan Heath Patterson1 3; Jamie L Allen2; Jessica R Sheldon4; David M Anderson1 2; Richard M. Caprioli1 2 5; Eric P Skaaar6 7; Jeffrey M. Spraggins1 2 7; 1Department of Biochemistry, Vanderbilt University, Nashville, TN; 2Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN 37205; 3Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; 4Vanderbilt Institute for Infection, Immunology, and Inflammation, Vanderbilt University, Nashville, TN; 5Department of Chemistry, Nashville, TN; 6Department of Pathology, Microbiology and Immunology, School of Medicine, Vanderbilt University, Nashville, TN; 7Department of Chemistry, Vanderbilt University, Nashville, TN

MOE am 09:50
Unravelling chemical mechanisms in microbial interactions by combining thin layer chromatography, ion mobility and MALDI imaging mass spectrometry; Andrée Moccant1; Christopher Kune1; Raphaël La Rocca1; Janina Oetjen2; Anhtho Arguelles Arias3; Marc Ongena3; Johann Far1; Gauthier Eppe2; Loic Quinton4; Edwin De Pauw1; 1University of Liege, MS Lab - GIGA, MolSys Research Unit, Liege, Belgium; 2Bruker Daltonik GmbH, Bremen, Germany; 3Gembloox Agro-Bio Tech, University of Liege, Gembloux, Belgium; 4University of Liege, Liege, Belgium

MOE am 10:10
A Galaxy-based meta-omic approach for characterizing microbiome functional dynamics via integrated metaproteomics and metatranscriptomics abundance analysis; Pratik Dilip Jagtap1; Praveen Kumar1; Marie A Crane2; Subina Mehta3; James E Johnson1; Thomas McGowan1; Magnus O Arnzen3; Francesco Delogu2; Ray Sajilga1; Srikant Verma4; Krishanpal Anamika5; Timothy J Griffin6; 1University of Minnesota, Minneapolis, MN; 2Macalester College: Private Liberal Arts College, St. Paul, Minnesota; 3Norwegian University of Environmental and Life Sciences, As, Norway; 4Persistent Systems Limited, Pune, India

MOF am: Biomarkers: Quantitative Analysis
Chair: Brian Rago (Pfizer)

MOF am 08:30
Development and qualification of a novel offline SPE and MRM method to quantify eicosanoids and related PUFAs; Monika Mital Kansal1; Veronica Anania2; Rod Mathews3; Olga Li1; 1Genentech, South San Francisco, CA

MOF am 08:50
Improving the Diagnosis and Treatment CKD-MBD using a UHPLC-HRMS Reference Measurement Procedure for Parathyroid Hormone; Candice Z. Ulmer1; Sarah Kingsley2; Bianca Smith2; Janet Thonkulpitak3; Hubert W. Vesper4; 1Centers for Disease Control and Prevention, Atlanta, GA; 2Battelle, Columbus, Ohio; 3Oak Ridge Institute for Science and Education (ORISE) Participant Program, Oak Ridge, Tennessee; 4Centers For Disease Control and Prevention, Atlanta, GA

MOF am 09:10
Quantitative MHC-I peptide measurement to support the development of cancer immunotherapeutic approaches using Parallel Reaction Monitoring; Vittoria Massafra1; Sabine Kux Van Geijtenbeek2; Martin Steegaifier3; Yvonne Anne Nagel4; Axel Ducet5; 1Roche Pharma Research and Early Development, Discovery Oncology, Roche Innovation Center Basel, Basel, Switzerland; 2Roche Pharma Research and Early Development, Pharmaceutical Sciences, Roche Innovation Center Basel, Basel, Switzerland; 3Roche Pharma Research and Early Development, Large Molecule Research, Roche Innovation Center Munich, Penzberg, Germany; 4Roche Pharma Research and Early Development, Discovery Oncology, Roche Innovation Center Basel, Basel, Switzerland

MOF am 09:30
A High Throughput Antibody-free Platform for Multiplexed, Sensitive Quantification of Protein Biomarkers in Complex Biomatrices; Bo An1; Timothy Sikorski1; Tu Jin Shi2; Yuqian Gao2; Jon Jacobs2; Matthew Szapacs1; 1GSK, Collegeville, PA; 2PNNL, Richland, WA

MOF am 09:50
A GCLP Quantitative Mass Spectrometry Workflow for Multiplexed Measurement of Protein Biomarkers in FFPE Tissues; Michael Schirm; Caprion Biosciences Inc., Montreal, QC
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<th>Session Title</th>
<th>Chair</th>
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<tr>
<td>MOG am 10:10</td>
<td>Applying high-throughput proteomics technology to discover biomarkers of liver disease</td>
<td>Lili Niu; Florian Meier; Philipp Geyer; Nicolai Jacob Wewer Albrechtsen; Alberto Santos Delgado; Rajat Gupta; Maja Thiele; Aleksander Krag; Janel Trebicka; Matthias Mann; *Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Copenhagen, Denmark; *Proteomics and Signal Transduction, Max Planck Institute of Biochemistry, Martinsried, Germany; Department of Clinical Biochemistry, Rigshospitalet, University of Copenhagen, Copenhagen N, Denmark; Department of Gastroenterology and Hepatology and OPEN, Odense Patient data Explorative Network, Odense University Hospital, Odense C, Denmark; Institute of Clinical Research, University of Southern Denmark, Odense C, Denmark; Department of Medicine I, University of Frankfurt, Frankfurt, Germany</td>
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<td>MOG am 08:30</td>
<td>Quantitative non-targeted LC/HRMS analysis for water and food monitoring</td>
<td>Anneli Kruve; Jaanus Liigand; Andrea Mizi Brunner; Tingting Wang; Jon R Sobus; Louis C Groff; Karin Kiefer; Juliane Hollender; Stockholm University, Stockholm, Sweden; University of Tartu, Institute of Chemistry, Tartu, Estonia; KWR Water Research Institute, Utrecht, Netherlands; Technical University of Denmark, Lyngby, Denmark; United States Environmental Protection Agency, Durham, NC; EAWAG, Duebendorf, Switzerland</td>
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<td>MOG am 08:50</td>
<td>Concurrent Electron and Proton Chemical Ionization of Polycyclic Hydrocarbons via the Liquid Sampling–Atmospheric Pressure Glow Discharge (LS–APGD) Ionization Source</td>
<td>R. Kenneth Marcus; Jacob R. Bills; Tyler J. Williams; Clemson University, Clemson, SC</td>
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<td>MOG am 09:00</td>
<td>Molecular Reconstruction and Analysis of Organic–Aerosol Composition from a High-alpine Glacier Ice Core Covering the Pre-industrial to the Present-day Transition</td>
<td>Alexander Vogel; Franziska Bachmeier; Anja Lauer; Katarzyna Artun; Urs Baltensperger; Elmad El Haddad; Margit Schwikowski-Gigar; Sasa Bjelic; Paul Scherrer Institute (PSI), Villigen PSI, Switzerland; Goethe-Universität, Frankfurt am Main, Germany; Paul Scherrer Institute (PSI), Villigen, Switzerland</td>
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<td>MOG am 09:30</td>
<td>On-Site Perfluorocarbon Tracer Detection with a Coded Aperture Miniature Mass Spectrometer</td>
<td>Kathleen L Horvath; Tanouir Aloui; Raul Vyas; Elettra Piccietto; Rafael Bento Serpa; Maria Luisa Sartorelli; Jason J Amsden; Jeffrey T. Glass; Roger P Sperline; M. Bonner Denton; Jesko Von Windheim; David Koester; Patrick Keelan; Yuri Zhilichev; Duke University, Durham, NC; Duke University, Durham; University of Arizona, Tucson, AZ 85351; PFT Technology LLC, Belleview, NY; Consultant, Durham, North Carolina</td>
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<td>MOG am 10:10</td>
<td>Empty Slot. Stay tuned for promoted selection to be made.</td>
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**MOG am: Environmental: Innovative Approaches and Instrumentation**

Chair: Achille Cappiello (University of Urbino)

**MOG am: Fundamentals: Ion Spectroscopy**

Chair: Jean-Yves Salpin (CNRS - University of Evry)

**MOH am 09:00** Novel LC - Infrared Ion Spectroscopy Approaches for the Structure Elucidation of Biomarkers | Fred A. M. G. Van Geenen; Udo F. Engelke; Rianne E. Van Outerstelp; Kas J. Houthuys; Giel Berden; Ron A. Wevers; Karlhen L. M. Coene; Jonathan Martens; Jos Oomens; *Radboud University, Institute for Molecules and Materials, FELIX Laboratory, Nijmegen, Netherlands; *Department of Laboratory Medicine, Translational Metabolic Laboratory, Radboud University Medical Center, Nijmegen, Netherlands; Van’t Hoff Institute for Molecular Sciences, University of Amsterdam, Amsterdam, Netherlands |

**MOH am 09:50** Intrinsic Effects of Fluorine Substitutions on the Structures and Glycosidic Bond Stabilities of Protonated Cytidine Analogues | Mary T Rodgers; Zachary J. Devereaux; Harrison A. Roy; Lucas A. Hamlow; Chenchen He; Yanlong Zhu; Erik O. Soley; Nathan A. Cunningham; Giel Berden; Jos Oomens; Wayne State University, Detroit, MI; *Radboud University, Institute for Molecules and Materials, FELIX Laboratory, Nijmegen, Netherlands |

**MOH am 09:10** Leveraging High-Resolution Mass Spectrometry and Cryogenic Vibrational Infrared Spectroscopy to Capture Intermediates in Small Molecule Activation: Applications to Nickel(II) | Evan H Perez; Sean C Edington; Fabian S Menges; Mark A Johnson; Yale University, New Haven, CT |

**MOH am 09:30** Reforming the Single-TurnAlpha Helix: Cold Ion Spectroscopy of Novel Cyclic Peptide Ions | John Lawler; Timothy Hill; David Fairlie; Timothy Zwier; Scott A. Mcluckey; Purdue University, West Lafayette, IN; University of Queensland, St Lucia, Australia; Sandia National Laboratories, Livermore, California |
UV/Vis Photodissociation Action Spectroscopy of Ionized DNA Components. Adenine and 9-Methyladenine Cation Radicals in the Gas-Phase; Shu R. Huang; Frantisek Turecek; University of Washington, Seattle, WA

Combined FAIMS, picosecond laser PD and ion trap MS reveals differences in the photostability of selected deprotonation isomers of FAD-; Samuel Marton; Ben I. McKinnon; Boris Ucur; Stephen J. Blanksby; Adam J. Trevitt; University of Wollongong, Wollongong, Australia; Queensland University of Technology, Brisbane, Australia
### MOA pm: Clinical Analysis : Applications

**Chair:** Therese Koal (Biocrates)

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<tr>
<td>MOA pm 02:30</td>
<td>Application of a Molecular Networking Approach combined with MetWork web server for Therapeutic Drug Monitoring and Toxicology</td>
<td>Emmanuel Bourgogne(^1,2); Christel Grondin(^3); Sophie Magréault(^4); Yann Beauxis(^5); Grégory Genta-Jouve(^6,8);  (^1)Université de Paris, Faculté de Pharmacie, Paris, France; (^2)APHP, Hôpital Saint Antoine, UF Suivi Thérapeutique du Médicament, Paris, France; (^3)APHP, Hôpital Lariboisière, UF Toxicologie, Paris, France; (^4)APHP, Hôpital Jean Verdier, UF Pharmacologie, Bondy, France; (^5)CNRS UMR8038, Paris, France; (^6)USR 3456 CNRS LEEISA, Cayenne, France</td>
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### MOA pm 02:50

**Title:** Tissue Identification and Diagnosis in Human Surgeries using the MasSpec Pen Technology

**Authors:** Jialing Zhang\(^1\); Marta Sans\(^2\); Rachel J. DeHoog\(^3\); Kyana Garza\(^4\); Mary King\(^5\); Clara L. Feider\(^1\); Alena Bensussan\(^6\); Michael F. Keating\(^1\); Anna C. Krieger\(^1\); Sunil P. Badali\(^1\); John Lin\(^1\); Wendong Yu\(^1\); Chandadeep Nagi\(^2\); Chris Pirko\(^1\); Kirian Brahmbhatt\(^2\); Thomas E. Milner\(^1\); Sadhna Dhingra\(^2\); George Van Buren\(^2\); Stacey A. Carter\(^2\); William E. Fisher\(^2\); Omar Barakat\(^2\); Raymond Grogan\(^2\); James Suliburk\(^2\); Livia S. Eberlin\(^3\); UT Austin, Austin, TX; \(^4\)Baylor College of Medicine, Houston, TX

### MOA pm 03:10

**Title:** Identification and characterization of antithrombin deficiency in patients using a targeted mass spectrometry based clinical chemistry test

**Authors:** Renee Ruhak\(^1\); Maria Eugenia De La Morena-Barrio\(^2\); Fred P.H.T.M. Romijn\(^1\); Mervin M. Pieterse\(^2\); Maarten P.J. Van Hoorn\(^1\); Javier Corral\(^2\); Christa M. Cobbaret\(^1\)

**Institutions:** \(^1\)Department of Clinical Chemistry and Laboratory Medicine, Leiden University Medical Center, Leiden, Netherlands; \(^2\)Servicio de Hematología y Oncología Médica, Hospital Universitario Morales Meseguer, Centro Regional de Hemodonación, Universidad de Murcia, IMIB-Arrixaca, Murcia, Spain

### MOA pm 03:30

**Title:** Multi-Center Assessment of Tumor Classification Reproducibility by MALDI Imaging

**Authors:** Soeren-Oliver Deininger\(^1\); Tobias Boskamp\(^1\); Christine Bollwein\(^2\); Rita Casadonte\(^3\); Petra Wandernoth\(^2\); Katharina Kriegsmann\(^1\); Mark Kriegsmann\(^2\); Jörg Kriegsmann\(^3\); Wilko Weichert\(^2\); Peter Schirrmacher\(^1\); Alice Ly\(^1\); Kristina Schwamborn\(^1\); Brucker Daltonik GmbH, Bremen, Germany; \(^2\)Institute of Pathology, Technical University Munich, Munich, Germany; \(^3\)Proteopath GmbH, Trier, Germany; \(^4\)Department of Hematology, Oncology and Rheumatology, University Hospital Heidelberg, Heidelberg, Germany; \(^5\)Institute of Pathology, University Hospital Heidelberg, Heidelberg, Germany

### MOA pm 03:50

**Title:** Fatty liver is more than “fat accumulation”: shotgun lipidomics of human non-alcoholic fatty liver disease and steatohepatitis

**Authors:** Olga Vvedenskaya\(^1\); Oskar Knittelfelder\(^2\); Alessandra Palladini\(^2\); Judith Wodke\(^3\); Tim Rose\(^4\); Eduardo Jacobo Miranda Ackerman\(^5\); Veera Raghavan Thangapandi\(^6\); Mario Brosch\(^5\); Edda Klipp\(^7\); Jochen Hamp\(^5,8\); Andrej Shevchenko\(^1\); \(^1\)Max Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG), Dresden, Germany; \(^2\)Paul Langerhans Institute Dresden of the Helmholtz Zentrum Munich at the University Clinic Carl Gustav Carus, Dresden, Germany; \(^3\)Humboldt University, Berlin, Germany; \(^4\)Technische Universität München, LipiTUM, Munich, Germany; \(^5\)Medizinischen Klinik 1 Bereich Gastroenterologie & Hepatologie, Universitätsklinikum Dresden, Dresden, Germany; \(^6\)Center for Regenerative Therapies, Dresden, Germany

### MOA pm 04:10

**Title:** Dilution in Situ for LC-MS/MS Workflows in Diagnostic Assays

**Authors:** Christine Gomez\(^1\); Matthew T Campbell\(^1\); Brian Rappold\(^1\); \(^1\)LabCorp, Raleigh, NC

### MOB pm: Exposomics, Toxicology, and Health Outcomes

**Chair:** Benedikt Warth (University of Vienna)

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<tr>
<td>MOB pm 02:30</td>
<td>Analyzing the Exposome: Perioperative environmental exposure to cyclohexanone during neonatal congenital cardiac surgery is associated with decreased neurodevelopmental outcomes</td>
<td>Allen Everett(^1); Jessie Buckley(^2); Greg Ellis(^3); Jun Yang(^4); David R Graham(^5); Eric Graham(^5); Johns Hopkins University School of Medicine, Baltimore, MD; (^2)Johns Hopkins University, Baltimore, MD; (^3)Johns Hopkins All Children's Hospital, St. Petersburg, 33701; (^4)Johns Hopkins School of Medicine, Baltimore, MD; (^5)Medical University of South Carolina, Department of Biochemistry and Molecular Biology, Charleston, SC</td>
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### MOB pm 02:50

**Title:** Metabolomics and Proteomics Analysis of the Effects of Vinclozolin Exposure in Utero on Dams and Fetuses

**Authors:** Alana Rister\(^1\); Ciro M. Amato\(^2\); Joshua P. Mogus\(^3\); Kimberly A. Kew\(^1\); Krista A. Mccoy\(^4\); East Carolina University, Greenville, North Carolina; \(^2\)National Institute of Environmental Health Sciences, Durham, North Carolina

### MOB pm 03:10

**Title:** Reactomics: using mass spectrometry as a reaction detector

**Authors:** Miao Yu\(^1\); Lauren Petrick\(^1\); \(^1\)Icahn School of Medicine at Mount Sinai, New York, NY

### MOB pm 03:30

**Title:** Targeted and Untargeted Screening of DNA Adducts in the Genome of Prostate Cancer Patients

**Authors:** Jingshu Guo\(^1\); Scott J. Walmsley\(^1\); Haoqing Chen\(^1\); Peter W. Villalta\(^1\); Paani Murugan\(^1\); Christopher J. Weight\(^1\); Robert J. Turesky\(^1\); \(^1\)University of Minnesota, Minneapolis, MN

### MOB pm 03:50

**Title:** Pan-albumin adductomics: Untargeted detection of electrophilic adducts at multiple residues of serum albumin for discovery and characterization of environmental exposures

**Authors:** Joshua W Smith\(^1\); Robert N...
MOD pm 04:10 Empty Slot. Stay tuned for promoted selection to be made.

MOD pm: Informatics: Metabolomics
Chair: Kendra Adams (Duke University)

MOD pm 02:30 CFM-ID 4.0: Substantially improved fragmentation algorithm and extended rules-based coverage of predicting ESI MS/MS spectra; Fei Wang1; Jaanus Liigand2, 3; David Arndt1; Russ Greiner1; David S Wishart1, 2; 1Department of Computing Science, University of Alberta, Edmonton, AB; 2Department of Biological Sciences, University of Alberta, Edmonton, AB; 3University of Tartu, Institute of Chemistry, Tartu, Estonia; 4Department of Computing Science, University of Alberta, Edmonton, AB T6G 2E8, Canada, Edmonton, AB

MOD pm 02:50 Developing a Data Processing Pipeline for Extending a Comprehensive Tandem Mass Spectral Library; Xianyu Yang1; Pedarsaz Neta1; Yuxue Liang1; Connie A. Remoroz1; Yamil Simón1; Kelly H. Telu1; Yuri A. Mirokhin1; Dmitrii V. Tchekhovskoi1; Alexey Mayorov1; Tytus D. Mak2; Lewis Y. Geer1; Stephen E. Stein1; 1National Institute of Standards and Technology, Gaithersburg, Maryland

MOD pm 03:10 Machine learning methods for METASPACE, an AI platform for spatial metabolomics; Theodore Alexandrov1, 2; Katja Ovchinnikova1; Lachlan Stuart1; Christopher M. Baxter Rath1, 3; Vitaly Kovalyev1; Veronika Saharuka1; Alexander Rakhlin4; Sergey Nikolenko5; 1EMBL – European Molecular Biology Laboratory, Heidelberg, Germany; 2Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; 3Omata Labs, San Diego, CA; 4Neuromation OU, Tallinn, Estonia; 5Steklov Institute of Mathematics, St.Petersburg, Russia

MOD pm 03:30 Combining biological and chemical information in compound annotation for untargeted metabolomics; Oliver Fiehn1; Clayton Bloziesz1; Dinesh K. Barupal1; Jacob Folz1; Ivan Blazenovic1; Tobias Kind1; Tomas Cajka1; Paolo Bonini1; Hiroshi Tsugawa1; 1UC Davis, Davis, CA; 2NGAlab, Tarragona, Spain; 3RIKEN Center for Sustainable Resource Science, Yokohama, Japan

MOD pm 03:50 Beyond the Top Hit: Extracting Unknown Structural Information from Hybrid Similarity Search Hit Lists; Brian T. Cooper1, 2; Tytus D. Mak2; Stephen E. Stein2; 1UNC Charlotte, Charlotte, NC; 2NIST, Gaithersburg, MD

MOD pm 04:10 Empty Slot. Stay tuned for promoted selection to be made.
MOE pm 02:30 Megadalton Mosaics: Assembling Molecular Information Piece by Piece using Charge Detection Mass Spectrometry; Conner C Harper; Evan R Williams; 1University of California, Berkeley, Berkeley, CA

MOE pm 02:50 Assessing DNA packaging in individual virophage virions using charge independent nano-mechanical MS; Christophe Masselon; Szu-Hsueh Lai; Sandra Jeudy; Bogdan Vysotsky; Kayva Clement; Lionel Bertaux; Marc Gely; Lucid Belmudes; Jean-Michel Claverie; Yohann Couté; Sébastien Hentz; Chantal Abergel; 1CEA, IRIG, Biologie à Grande Echelle, Grenoble, France; 2Aix-Marseille University, CNRS UMR 7283, Marseille, France; 3Université Grenoble Alpes, CEA, LETI, Grenoble, France

MOE pm 03:10 Charge Detection Mass Spectrometry Measurements of Exosomes and other Extracellular Particles Enriched from Bovine Milk; Brooke A Brown; Xuyao Zeng; Aaron Todd; Lauren Frances Barnes; Jonathan Winstone; Jonathan C. Trinidad; Milos V. Novotny; Martin F. Jarrold; David E. Clemmer; 1Indiana University, Bloomington, IN

MOE pm 03:30 Mass and charge distributions of entire amyloid fibers by charge detection mass spectrometry: mapping heterogeneity and polymorphism; Mohammad Abdul Halim; Jonathan Pansier; Philippe Dugourd; Vincent Forge; Rodolphe Antoine; 1University of Arkansas Fort Smith, Fort Smith, AR; 2Nuffield Department of Clinical Neurosciences, Oxford University, Oxford, United Kingdom; 3Institut Lumière Matière CNRS et Université Lyon 1, LYN, France; 4Laboratoire Chimie et Biologie des Métaux CEA-Grenoble, Grenoble, France

MOE pm 03:50 Resolving heterogeneous macromolecular assemblies by Orbitrap-based (UHMR) single particle charge-detection mass spectrometry (CD-MS); Tobias P. Wörner; Joost Snijders; Antonette Bennett; Mavis Abugande-McKenna; Thomas W. Powers; Olga F. Friese; Alexander A. Makarov; Albert J.R. Heck; 1Biomolecular Mass Spectrometry and Proteomics, Faculty of Science, Utrecht University, 3584 CH Utrecht, Netherlands; 2Netherlands Proteomics Center, Padualaan 8, Netherlands; 3Department of Biochemistry and Molecular Biology, Center for Structural Biology, the McKnight Brain Institute, 1200 Newell Drive, Gainesville, FL 32610; 4BioTherapeutics Pharmaceutical Sciences, Pfizer, Inc, Chesterfield, MO 63017; 5Thermo Fisher Scientific, Bremen, Germany

MOE pm 04:10 From Human Nucleosomes to Virus-Like Particles: Multiplexing the Orbitrap to Readout Individual Ion Mass Spectra; Jared Kafader; Rafael D Melani; Luis Schachner; Kenneth R Durbin; Bon Ikwuagwu; Bryan P Early; Ryan T Fellers; Steven C Beu; Vlad Zabrousok; Joshua T Maze; Deven L Shinholt; Ping F. Yip; Danielle Tullman-Eerce; Michael W. Senko; Philip D. Compton; Neil L. Kelleher; 1Northwestern University, Evanston, IL; 2S.C. Beu Consulting, Austin, Texas; 3Thermo Fisher Scientific, San Jose, CA; 4Thermo Fisher Scientific, Austin, TX

MOF pm 02:30 Mapping ADP-ribosylation using Activated Ion Electron Transfer Dissociation (AI-ETD); Sara C Buch-Larsen; Ivo A Hendriks; Jean M Lodge; Martin Ryker; Benjamin Furtwängler; Evgenia Shishkova; Michael S. Westphall; Joshua J Coon; Michael L Nielsen; 1Novo Nordisk Foundation Center for Protein Research, København, Denmark; 2Equal contribution, .., Denmark; 3University of Wisconsin-Madison, Madison, Wisconsin

MOF pm 02:50 Identification and characterization of a new protein post-translational modification, lysine lactylation, by mass spectrometry-based proteomics approaches; Di Zhang; Zhanyun Tang; He Huang; Guolin Zhou; Mathew Perez-Neut; Robert G. Geoder; Lev Becker; Yingming Zhao; 1Ben May Department for Cancer Research, The University of Chicago, Chicago, Illinois; 2Laboratory of Biochemistry and Molecular Biology, The Rockefeller University, New York, NY

MOF pm 03:10 From single cell to single embryo: Unraveling protein phosphorylation dynamics of the early cell cycle; Juan M Valverde; Liliana Krasińska; Daniel Fisher; Albert J.R. Heck; Puck Knipscheer; Maarten Atellaar; 1Biomolecular Mass Spectrometry and Proteomics, Bijvoet Center for Biomolecular Research and Utrecht Institute for Pharmaceutical Sciences, Utrecht, Netherlands; 2Netherlands Proteomics Center, Utrecht, Netherlands; 3Montpellier Institute of Molecular Genetics, Montpellier, France; 4Oncode Institute, Hubrecht Institute–KNAW and University Medical Center, Utrecht, Netherlands

MOF pm 03:30 Quantification of thermal stability of intact proteoforms using quantitative top-down proteomics; Kellye A Cupp-Sutton; Thomas Welborn; Si Wu; 1University of Oklahoma, Norman, OK

MOF pm 03:50 Quantitative Top-Down Proteomics reveals the Distinct Substrate Specificity of p300 and CBP; Tao Wang; Matthew V. Holt; Nikit Venishetty; Nicolas L. Young; 1Baylor College of Medicine, Houston, TX; 2Rice University, Houston, TX; 3Baylor College of Medicine, Houston

MOF pm 04:10 Empty Slot. Stay tuned for promoted selection to be made.
MOG pm: Stable Isotope Labeling: Applications
Chair: Matthew Foster (Duke University)

MOG pm 02:30 Single injection LC-HRMS large-scale quantitative metabolomics using multipoint internal calibration and on-demand produced multideuterated metabolites; Kathleen Rousseau1; Jessica Michieletto1; Yu Min Kwi1; Sophie Feuillatre2; Grégory Pieters2; Christophe Junot1; François Fenaille1; Annelaure Damont1; 1Université Paris-Saclay, CEA, INRAE, Médicaments et Technologies pour la Santé (MTS), MetaboHUB, Gif-sur-Yvette, France; 2Université Paris-Saclay, CEA, INRAE, Médicaments et Technologies pour la Santé (MTS), Gif-sur-Yvette, France

MOG pm 02:50 Detection of Lipogenesis at Very High Sensitivity Using Orbitrap Gas Chromatography High-resolution Mass Spectrometry; Xiaorong Fu1; Stanislaw Deja1; Justin Fletcher1; Norma Anderson1; Matthew Mitsche1; Goncalo Vale1; Jeffrey Mcdonald1; Jay Horton1; Shawn Burgess1; 1UT Southwestern Medical Center, Dallas, TX

MOG pm 03:10 Use of stable isotope-labeled peptidic drugs to facilitate metabolite identification for sports drug testing purposes; Mario Thevis1; Andreas Thomas1; 1German Sport University, Cologne, Germany

MOG pm 03:30 Methylation dynamics of histone H3.3K27me3 in pluripotency and differentiation of embryonic stem cells; Yekaterina Kori1; Simone Sidoli1,2; Zuo-Fei Yuan1,2; Benjamin A. Garcia1; 1University of Pennsylvania, Philadelphia, PA; 2Albert Einstein College of Medicine, The Bronx, NY; 2St. Jude Children’s research hospital, Memphis, TN

MOG pm 03:50 In vivo Protein Turnover Rates Across the Proteome for Various Mouse Tissues; Zach Rolls1; Brian L Frey1; Xudong Shi2; Yoshitaka Kawai2; Lloyd M Smith1; Nathan V Welham2; 1Department of Chemistry, University of Wisconsin-Madison, Madison, WI; 2Department of Surgery, University of Wisconsin-Madison, Madison, WI

MOG pm 04:10 Analysis of Isotopically-Depleted Proteins Derived from Bacterial Cells by 21 Tesla Fourier Transform Ion Cyclotron Resonance Mass Spectrometry; Zeljka Popovic1; Lissa C. Anderson2; Xuepei Zhang3; David S. Butcher2; Greg T. Blakney2; Roman Zubarev3; Christopher L. Hendrickson1,2; Alan G. Marshall1,2; 1Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL; 2National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; 3Karolinska Institute, Solna, Sweden

MOH pm: Fundamentals: Ion Activation and Dissociation
Chair: John Stutzman (The Dow Chemical Company)

MOH pm 02:30 Desalting proteins using infrared photoactivation; Jean M Lodge1; Michael S Westphall1; Joshua J Coon1; 1University of Wisconsin, Madison, WI

MOH pm 02:50 Gas-phase separation and concentration of phosphatidylcholine lipids using charge inversion ion/ion reactions enabled on an FT-ICR mass spectrometer; Jonathan T Specker1; Boone M. Prentice1; 1University of Florida, Gainesville, FL

MOH pm 03:10 CID Tandem MS and Traveling Wave IMS to Investigate Non-Covalent Interactions for Asymmetric Catalysis; Dr. Ulrike Warzok1; Banruo Huang1; Dr. Anthony T. Iavarone1; Prof. F. Dean Toste1; 1University of California, Berkeley, Berkeley, CA

MOH pm 03:30 Simple and minimally invasive SID devices for native mass spectrometry; Dalton Snyder1; Erin Panczyk1; Ben Jones1; Arpad Somogyi1; Desmond Kaplan2; Vicki Wysocki1; 1The Ohio State University, Columbus, OH; 2KapScience LLC, TEWKSBURY, MA

MOH pm 03:50 Selective gas-phase ion/ion chemistries for the structural elucidation of complex lipids in direct infusion workflows; Caitlin E. Randolph1; De’shovon M. Shenault1; Kimberly C. Fabijanczuk1; Reuben S. E. Young2; Stephen J. Blanksby2; Scott A. Mcluckey1; 1Purdue University, West Lafayette, IN; 2Queensland University of Technology, Brisbane, Australia

MOH pm 04:10 UVPD-FTICR-2DMS: Expanding the toolbox for biomolecule analysis; Alina Theisen1; Christopher A. Wootton1; Anisha Haris1; Tomos E. Morgan1; Yuko Lam1; Sean Ellacott1; Sebastien Perrier1; Mark P. Barrow1; Peter B. O’Connor1; 1University of Warwick, Coventry, United Kingdom
# TUESDAY AM ORALS

## TOA am: Instrumentation: New Developments in Ionization and Sampling: In Memory of Burnaby Munson

**Chair:** Jeffrey McGuire (U.S. Army CCDEVCOM Chemical Biological Center)

<table>
<thead>
<tr>
<th>Time</th>
<th>Title</th>
<th>Authors</th>
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<tbody>
<tr>
<td>08:30</td>
<td>A Novel NanoESI-Microreactor Ionization Source for Microwave-Assisted Bottom-Up Proteomics</td>
<td>Maria E Rivera, Steven J Ray, University at Buffalo, Buffalo, NY</td>
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<tr>
<td>08:50</td>
<td>On-demand ionization for miniature mass spectrometry analysis system</td>
<td>Junhan Wu, Wenpeng Zhang, Zheng Ouyang, Tsinghua University, Beijing, China, Purdue University, West Lafayette</td>
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<td>09:10</td>
<td>Electron Ionization LC-MS and GC-MS Combined Instrument Using Single MS</td>
<td>Alexander B. Fialkov, Avi Amirav, Tel Aviv University, Tel Aviv, Israel</td>
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<td>09:30</td>
<td>Spray-cappillary Based Capillary Electrophoresis Mass Spectrometry Analysis of Metabolites in Live Cells</td>
<td>Lushuang Huang, Zhe Wang, Mulin Fang, Drew King, Cupp-Sutton Kelly, Si Wu, University of Oklahoma, Dept. of Chem &amp; Biochem, Norman, OK, University of Oklahoma, Norman, OK</td>
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<tr>
<td>09:50</td>
<td>New Approaches for Efficient Sampling and Ionization in High-Resolution Imaging Using Nanospray Desorption Electrospray Ionization (nano-DESI) Mass Spectrometry</td>
<td>Ruichuan Yin, Daisy M Unshuay Vila, Daniela Mesa Sanchez, Purdue University, West Lafayette, IN</td>
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<td>10:10</td>
<td>Boosting Ion Signal Levels with cVSSI for MS/MS and MSn of Biopolymers</td>
<td>Kushani U Attanayake, Chong Li, Daud Sharif, Sandra N Majuta, Ahmad Kiani Karanjii, Anthony Debastiani, Peng Li, Stephen J Valentine, West Virginia University, Morgantown, WV</td>
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## TOB am: Lipidomics: New MS Technologies and Applications

**Chair:** Komal Kedia (Merck)

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<th>Time</th>
<th>Title</th>
<th>Authors</th>
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<tr>
<td>08:30</td>
<td>An automated protocol for liquid-liquid extraction of blood plasma polar metabolites and lipids for mass spectrometry</td>
<td>Tobias Marcus Maile, Sudha Gollapudi, Aleksandr Gaun, Ngoc Vu, José Zaraval-Solorio, Ganesh Kolumam, Fiona E. Mccallister, Rob Keyser, Bryson D. Bennett, Calico LLC, South San Francisco, CA</td>
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<td>08:50</td>
<td>High-throughput and robust nanoflow chromatography combined with trapped ion mobility spectrometry and PASEF for in-depth lipidomics from 1µL human plasma</td>
<td>Catherine G. Vasilopoulos, Nicolai Bache, Ole Hoerning, Philipp E. Geyer, Karolina Sulek, Andreas-David Brunner, Dmitry Voytik, Sanjib Meitel, Aiko Barsch, Matthias Mann, Florian Meier, Max Planck Institute of Biochemistry, Martinsried, Germany, Evosep Biosystems, Odense, Denmark, NNF Center for Protein Research, Copenhagen, Denmark, PREMIER Biosoft, Indore, India, Bruker Daltonik GmbH, Bremen, Germany</td>
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<td>09:10</td>
<td>A workflow to link lipid structures with biological and metadata utilizing novel visualization and clustering tools</td>
<td>Melanie Odenkirk, Phyo Phyo Kyaw Zin, Jeremy Ash, David Ref, Denis Fourches, Erin S. Baker, Department of Chemistry, North Carolina State University, Raleigh, North Carolina, Department of Statistics, North Carolina State University, Raleigh, North Carolina, Department of Biological Sciences, North Carolina State University, Raleigh, North Carolina</td>
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<td>09:30</td>
<td>Multinozzle Emitters for Shotgun Lipidomics</td>
<td>Na Pi Parra, Maoyin Li, Pan Mao, Daojing Wang, Newomics Inc., Berkeley, CA</td>
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<td>09:50</td>
<td>Untangling and Quantifying Isomeric Molecular Gangliosides using High Throughput Structures for Lossless Ion Manipulation-MS Analyses</td>
<td>Kelly Wormwood, James R. Arndt, Liulin Deng, Anisha Yadav, Stephen Krufka, Daniel Debdor, Laura Maxon, Kim Ekroos, MOBILion Systems Inc., Chadds Ford, PA, Lipidomics Consulting Ltd, Esbo, Finland</td>
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<td>10:10</td>
<td>ANALYSIS BY LC-MS/MS OF LIPIDS EXTRACTED USING TRIZOL REAGENT</td>
<td>Rahul Deshpande, Nathen Bopp, William Russell, Mass Spectrometry Facility, University of Texas Medical Branch (UTMB), Galveston, TX</td>
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</table>
The landscapes of antigen-engaged nanobody proteomes; Zhe Sang1; Yufei Xiang1; Dina Schneidman2; Yi Shi1; 1University of Pittsburgh, Pittsburgh, PA; 2Hebrew University of Jerusalem, Jerusalem, Israel

TOC am 09:50

Competitive SEC affinity separation for identification of antibody modifications impacting binding to target protein; Rachel Luqing Shi1; Gang Xiao1; Thomas M Dillon1; Arnold Mcauley1; Margaret S Ricci1; Pavel V. Bondarenko1; 1Bristol-Myers Squibb, Princeton, NJ; 2Bristol-Myers Squibb, Redwood City, CA

TOC am 10:10

Deep learning improves sensitivity and specificity of peptide identification in immunopeptidomics; Kai Li1, 2; Bo Wen1, 2; Bing Zhang1, 2; 1Lester and Sue Smith Breast Center, Baylor College of Medicine, Houston, TX 77030; 2Department of Molecular and Human Genetics, Baylor College of Medicine, Houston, TX 77030

TOD am: Informatics: Multiomics Integration and Applications

Chair: Amina Woods (NIDA IRP, NIH)

TOD am 08:30

Integration of metabolomics & proteomics profiles of NGLY1 deficiency plasma and cellular models to identify molecular phenotypes; Songjie Chen1; Guangwen Wang1; Xiaotao Shen1; Daniel Hornberg1; Michael Snyder1; 1Stanford University, Stanford, CA

TOD am 08:50

DMDB: A database for drug interactions, metabolism and mechanism of action based on integrative Omics; Raghav Sehgal1; Rebecca Cardone1; Richard Martyn Williams1; Xiaojian Zhao1; Qishi Sun1; Surbhi Poddar2; Richa Mudga2; Richard Schneider2; Richard G. Kibbey1; 1Yale University, New Haven, CT; 2Elucidata, Delhi, India; 3NIH/NCATS, Rockville, MD

TOD am 09:10

Utilizing a Proteogenomic Pipeline to Verify Novel Transcription Events in Neurological Research; Conor C Jenkins1, 2; Benjamin Orsburn2, 3; Miranda Darby1; 1Hood College, Frederick, MD; 2Proteomic Und Genomic Sciences, Glen Rock, PA; 3University of Virginia School of Medicine, Charlottesville, VA

TOD am 09:30

Aqueous Humor Metabolite Profile of Pseudoexfoliation Glaucoma is Distinctive; Ciara Myer1; Leila Abdelrahman1; Santanu Banerjee1, 2; Ram Khatri3; Matthew E. Merritt4; Anna K. Junk1; 1, 2, 3, 4Worcester Polytechnic Institute, Worcester, MA; 2Hood College, Frederick, MD; 3Department of Ophthalmology and Visual Science, University of Maryland, Baltimore, MD; 4Department of Ophthalmology, University of Virginia, Charlottesville, VA

TOD am 09:50

Automating the Analysis of Multi-Omics Data to Accelerate Breeding and Crop Protection Programs; Joe Shambaugh1; Benjamin J Adamczyk2; Thomas Hartsch3; Peter Haber4; 1Genedata Inc, Lexington, MA; 2Genedata, Lexington, MA; 3Genedata AG, Basel, Switzerland; 4Genedata GmbH, Munich, Germany

TOD am 10:10

Advantages of multipronged search and processing tools to analyze TMT-labeled and XL-MS datasets; Ying Zhang1; Zhihui Wen1; Michael Washburn1; Laurence Florens1; 1Stowers Institute for Medical Research, Kansas City, MO

TOD am: Therapeutic Proteins, Antibodies, and Antibody/Drug Conjugates

Chair: M. Violet Lee (Genentech)

TOD am 08:30

In vitro and in vivo biotransformation studies by intact mass analysis for novel biotherapeutics; Yunan Wang1; Mei Han1; Brooke M. Rock1; Dan A. Rock1; 1Amgen, SSF, CA

TOD am 08:50

Accelerated sequence identification of functional antibodies from high throughput human B-cell screens using reversed immunopanopatute / HR LC-MS2: Eberhard Durr1; Yaping Liu1; Arthur Fridman1; Zhifeng Chen1; Nicole Sullivan1; Kristin Geddes1; Aimin Tang1; Brian Squadron1; Paul Zuck1; 1Merck Research Laboratories, West Point, PA; 2Merck Research Laboratories, Rahway, NJ

TOD am 09:10

Mapping Binding Epitopes of Bispecific Antibody with Integrated Mass Spectrometry-based Protein Footprinting Approaches; Richard Huang1; Feng Wang2; Matthew Wheeler2; Bryant Chau2; Jia Dong2; Winse Morishige2; Natalie Bezman2; Pavel Strop2; Arvind Rajpal2; Olafur Gudmundsson1; Guodong Chen1; 1Bristol-Myers Squibb, Princeton, NJ; 2Bristol-Myers Squibb, Redwood City, CA

TOD am 09:30

The landscapes of antigen-engaged nanobody proteomes; Zhe Sang1; Yufei Xiang1; Dina Schneidman2; Yi Shi1; 1University of Pittsburgh, Pittsburgh, PA; 2Hebrew University of Jerusalem, Jerusalem, Israel

TOD am 09:50

Competitive SEC affinity separation for identification of antibody modifications impacting binding to target protein; Rachel Luqing Shi1; Gang Xiao1; Thomas M Dillon1; Arnold Mcauley1; Margaret S Ricci1; Pavel V. Bondarenko1; 1Bristol-Myers Squibb, Princeton, NJ; 2Bristol-Myers Squibb, Redwood City, CA

TOD am 10:10

Deep learning improves sensitivity and specificity of peptide identification in immunopeptidomics; Kai Li1, 2; Bo Wen1, 2; Bing Zhang1, 2; 1Lester and Sue Smith Breast Center, Baylor College of Medicine, Houston, TX 77030; 2Department of Molecular and Human Genetics, Baylor College of Medicine, Houston, TX 77030
TOF am: Art, Archaeology, and Paleontology
Chair: Timothy Cledand (Smithsonian Institution)

TOF am 08:30 Tandem MS identifies unexpected components in the ground layer of paintings from the Danish Golden Age; Fabiana Di Gianvincenzo1; Meaghan Mackie1,2; Troels Filtenborg1; Cecil Krakup Andersen3; Madeleine Ernst1; Jørgen Wadum1; Enrico Cappellini1; 1GOBE institute, University of Copenhagen, Copenhagen, Denmark; 2Novo Nordisk Foundation Center for Protein Research – University of Copenhagen, Copenhagen, Denmark; 3National Gallery of Denmark, Copenhagen, Denmark; 4Center for Newborn Screening, Department of Congenital Disorders, Statens Serum Institut, Copenhagen, Denmark

TOF am 08:50 Trace level top down proteomics analysis: application to the study of Gainsborough drawings; Francesca Galluzzi1; Julie Arslanoglou2; Catherine Rawlins1; Stephane Clavero1; Federica Pozzi2; Reba F. Snyder3; Caroline Tokarski1; 1Institute of Chemistry and Biology of Membrane and NanoObjects, UMR CNRS 5248, Proteome Platform, University of Bordeaux, Bordeaux, France; 2Department of Scientific Research, The Metropolitan Museum of Art, New York, 10028; 3Thaw Conservation Center, The Morgan Library & Museum, New York, 10016

TOF am 09:10 Bioarchaeological Proteomic Analysis of Skin Samples from an Ancient Egyptian Child Mummy; Prathiba Ravishankar1; Dylan Multari1; Ronika K Power1; Paul A. Haynes1; 1Macquarie University, North Ryde, Sydney, Australia

TOF am 09:30 Large-scale Palaeoproteogenomics to explore the phylogenetic tree of Elephantidae; Patrick Leopold Ruether1; Simon Rasmussen1; Immanuel Husic1; Marianne Dehasque2; Love Dalén2; Jesper V Olsen3; 1NNF Center for Protein Research University of Copenhagen, Copenhagen, Denmark; 2Center for Palaeogenetics, Stockholm, Sweden

TOF am 09:50 Resurrecting the Protein Sequence from Hadrosauridae Egg Shells; Emily R Sekera1; Connor Gould1; Nerith Rocío Elejalde Cadena2; Abel Moreno Cárcamo2; Troy D Wood1; 1University at Buffalo, Buffalo, NY; 2Universidad Nacional Autónoma de México, Coyoacán, Mexico

TOF am 10:10 GrandPep, a novel software for computational reconstruction of ancient protein sequences; Petra Gutenbrunner1; Frido Welker2; Jazmin Ramos-Madrigal2; Assa Yeroslaviz; Juergen Cox1; 1Max Planck Institute of Biochemistry, Martinsried, Germany; 2University of Copenhagen, Evolutionary Genomics Section, Globe Institute, Copenhagen, Denmark

TOF am: Covalent Labeling and Chemical Crosslinking
Chair: Fabio Gozzo (IQ - University of Campinas)

TOF am 08:30 A novel straightforward in vivo cross-linking mass spectrometry strategy for proteome-wide studies; Lucienne Nouchikian1; Martial Rey1; Jonathan Dhenin1; Youxin Kong1; Guillaume Duménil1; Julia Chamot-Rooke1; 1Institut Pasteur, Paris, France

TOF am 08:50 A combination of top-down and cross-linking mass spectrometry illuminates the pairing of PSII-LHCII supercomplexes across thylakoid membranes; Pascal Albanese1,2,3; Sem Tamara1,4; Cristina Pagliano1; Richard Scheltema1,5; 1Applied Science and Technology Department–BioSolar Lab, Politecnico di Torino, Torino, Italy; 2Biomolecular Mass Spectrometry and Proteomics, Bijvoet Center for Biomolecular Research and Utrecht Institute for Pharmaceutical Sciences, Utrecht, Netherlands; 3Netherlands Proteomics Center, Utrecht, Netherlands; 4Biomolecular Mass Spectrometry and Proteomics, Utrecht Institute for Pharmaceutical Sciences, Utrecht University, Utrecht, Netherlands

TOF am 09:10 In-depth characterisation of UV-induced cross-linking in a model protein-RNA complex: Implications for structural proteomics of ribonucleoproteins; Chris P. Sarnowski1; Anna Knörlein2; Tebbe De Vries3; Michael Götz1; Ruedi Aebersold1,4; Frédéric H-T Allain1; Jonathan Hall2; Alexander Lettner1; 1Institute of Molecular Systems Biology, Department of Biology, ETH Zürich, Zürich, Switzerland; 2Institute of Pharmaceutical Sciences, Department of Chemistry, ETH Zürich, Zürich, Switzerland; 3Institute of Biochemistry, Department of Biology, ETH Zürich, Zürich, Switzerland; 4Faculty of Science, University of Zürich, Zürich, Switzerland

TOF am 09:30 Stitching the synapse: untargeted cross-bridging mass spectrometry (XL-MS) into resolving synaptic protein interactions; Miguel A Gonzalez-Lozano1; Frank Koopmans1; Patrick F Sullivan2; Jonas Protze3; Gerd Krause1; Matthijs Verhage1; Ka Wan Li1; Fan Liu1; August B Smit1; 1Vrije University Amsterdam, Amsterdam, Netherlands; 2Karolinska Institutet, Stockholm, Sweden; 3Leibniz-Forschungsinstitut für Molekulare Pharmakologie, Berlin, Germany

TOF am 09:50 Using In-Cell Fast Photochemical Oxidation of Proteins to Observe Changes in Gleevec's Drug Target Engagement in Triple Negative Breast Cancer; Emily E Chea1; Lisa Jones2; 1University of Maryland Baltimore, Baltimore, MD; 2University of Maryland, Baltimore, MD

TOF am 10:10 First Draft of the Human Lysosomal Interactome by Cross-Linking Mass Spectrometry Reveals Novel Interactions and Structures; Jasjot Singh1; Hadeer Elhabashy2; Volkmar Gieselmann1; Oliver Kohlbacher2; Dominic Winter3; 1Institute of Biochemistry and Molecular Biology - University Bonn, Bonn, Germany; 2Institute
TOH am: Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, and Supplements
Chair: Ann Knolhoff (FDA)

TOH am 08:30 Inhibitory mechanism and kinetics of active components of licorice Glycyrrhiza uralensis Fisch. ex DC. on human cytochrome P450 enzymes; Luaying Chen¹, ²; Laura Tyler³; Dejan S. Nikolic²; Guannan Li⁴; Guido F. Pauli⁵; Richard B. van Bremen¹, ², ³; Linus Pauling Institute, College of Pharmacy, Oregon State University, Corvallis, OR; ²UIC/NIH Center for Botanical Dietary Supplements Research, Chicago, IL

TOH am 08:50 Development of MS-based detection method for cashew proteins in an oil matrix based on a comprehensive protein database; Shimin Chen¹; Melanie Downs¹; University of Nebraska-Lincoln, Lincoln, NE

TOH am 09:10 Liquid is better: liquid AP-MALDI MS high-throughput analysis for food adulterations, diagnostics and early animal disease detection; Cristian Piras¹; Barney Jones²; Nick Taylor³; Oliver J Hale⁴; Michael Morris⁵; Chris Reynolds⁵; Rainer Cramer¹; Department of Chemistry, University of Reading, Reading, United Kingdom; ²Centre for Dairy Research (CEDAR), School of Agriculture, Policy and Development, University of Reading, Reading, United Kingdom; ³Waters Corporation, Wilmslow, United Kingdom

TOH am 09:30 Automated chiral analysis of free amino acids in fermented foods by trapped ion mobility-mass spectrometry; Jonas M. Will¹; Arne Behrens¹; Marcel Macke¹; C. Derrick Quarles Jr.²; Uwe Karst⁴; University of Muenster, Institute of Inorganic and Analytical Chemistry, Muenster, Germany; ²Elemental Scientific, Inc. (ESI), Omaha, Nebraska

TOH am 09:50 Integrating Metabolomics and NIR Spectral Data for Fruit Quality Assessment and Their Applications in Apple Breeding: Kevin Hooton¹; Rachael Leblanc¹; David Liscombe¹; Vineland Research and Innovation Centre, Vineland Station, Ontario

TOH am 10:10 Empty Slot. Stay tuned for promoted selection to be made.

TOH am: Homeland Security, Defense, and Extreme Environments: Developments and Applications
Chair: Trevor Glaros (CCDC Chemical Biological Center)

TOH am 08:30 Quantitative proteomic-based approaches development to study the human proteome changes during real space missions and ground-based experiments; Alexey Kononikhin¹, ²; Alexander Brzhovozvskiy¹, ²; Anna Bugrova³; Maria Indekyna³; Daria Kashirina³; Anna Ryabokon²; Ludmila Pastushkova²; Igor Popov⁴; Irina Larina²; Christoph H. Borchers¹, ⁵; Eugene (evgeny) Nikolaev¹; ²Skolkovo Institute of Science and Technology, Moscow, Russia; ³Institute of Biomedical Problems, Russian Academy of Sciences, Moscow, Russia; ⁴Emanuel Institute for Biochemical Physics, Russian Academy of Sciences, Moscow, Russia; ⁵Moscow Institute of Physics and Technology, Dolgoprudny, Russia; ²McGill University, Montreal, QC

TOH am 08:50 Combination of Surface-Enhanced Raman Spectroscopy and Paper Spray Ionization on Portable Instrumentation for On-Site Drug Analysis; Ashley Stelmack¹; Christopher C. Mulligan¹; William L. Fatigante¹; Daniel S. Burr¹; Noah W. McClurg¹; Trevor J. McDaniel¹; Jemima Larney¹; Jamie R. Wieland¹; Jeremy D. Driskell¹; Jun-Hyun Kim¹; Illinois State University, Normal, IL

TOH am 09:10 Development of a drone-based TF-SPME water sampler for the on-site screening of environmental pollutants and protection at remote locations; Jonathan J Grandy¹; Virginia Galpin²; Varoon Singh²; Janusz Pawliszyn¹; University of Waterloo, Waterloo, ON; ²University of Waterloo, Waterloo, ON

TOH am 09:30 Identification of Diagnostic Markers Indicative of Exposure to Energetic Materials Using Mass Spectrometric Techniques and Random Forest Classification; Cameron Longo¹; Samira Beyramysoltan¹; Rabi A. Musah¹; University at Albany - SUNY, Albany, NY

TOH am 09:50 The Advantages of Two-Dimensional Mass Spectrometry Analysis of Agrochemicals in Environmental Samples; Bryan P. Marzullo¹; Tomos E. Morgan¹; Christopher A. Wootton¹; Simon J. Perry²; Mansoor Saeed²; Mark P. Barrow³; Peter B. O'Connor³; University of Warwick, Coventry, United Kingdom; ²SYNGENTA, Bracknell, United Kingdom

TOH am 10:10 On-demand Atmospheric Arc Ionization for Analyzing Swabbed Samples Using Miniature Mass Spectrometer; Ningxi Li¹; Zhijun Cai¹; Wenbo Cao¹; Huarong Gu¹; Zheng Ouyan¹; State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China
### TOA pm: Instrumentation: Portable and Transportable Mass Spectrometers

**Chair:** Donna Hollinshead

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<td>02:30</td>
<td>Intelligent Handheld Mass Spectrometer for On-Site Analysis; Bin Jiao¹; Xinwei Liu¹; Jiejun Bu²; Huimin Ye¹; Zheng Ouyang¹; ²Tsinghua University, Beijing, China; ²PURSPEC Technologies, Beijing, China</td>
<td>TOA pm 02:30</td>
<td>³University of Florida, Gainesville, FL; ³University of Arizona, Tucson, AZ 85721</td>
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<td>02:50</td>
<td>2D MS/MS Scans on Benchtop and Portable Ion Trap Mass Spectrometers; Lucas Szalwinski¹; Dylan T Holdren¹; R. Graham Cooks¹; ²Purdue University, West Lafayette, IN</td>
<td>TOA pm 02:50</td>
<td>³University of Arizona, Tucson, AZ 85721</td>
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<td>03:10</td>
<td>Measurement of THC in Exhaled Breath after Marijuana smoking: Exploring The Potential of a Transportable LC-CMS System; Olof Beck¹; Jack Henion²; Sabina Seferaj³; Peter Stambekc⁴; ³Department of Clinical Neuroscience, Stockholm, Sweden; ²Advin Inc., Ithaca, NY; ³Karolinska University Hospital, Stockholm, Sweden; ⁴Munkplast AB, Uppsala, Sweden</td>
<td>TOA pm 03:10</td>
<td>³University of Arizona, Tucson, AZ 85721</td>
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<td>03:30</td>
<td>Design considerations for a cycloidal mass analyzer; Elettra L. Piacentino¹; Kathleen Horvath¹; Maria Luisa Sartorelli²; Tanouir Aloui³; Raúl Vyas⁴; Rafael Bento Serpa⁵; Charles B. Parker⁶; Yuriy Zhitichev⁷; Roger P. Sperline⁷; Robert Kingston⁸; Scott Tilden⁸; Justin Keogh⁹; Jeffrey T Glass¹⁰; Jason J Amsden¹¹; M. Bonner Denton¹²; ¹Duke University, Durham, NC; ²Universidade Federal de Santa Catarina, Trindade, Brazil; ³Duke University, Durham, North Carolina; ⁴Consultant, Durham, North Carolina; ⁵University of Arizona, Tucson, AZ; ⁶University of Arizona, Tucson, AZ 85351</td>
<td>TOA pm 03:30</td>
<td>³University of Arizona, Tucson, AZ 85721</td>
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<td>04:01</td>
<td>Mars Organic Molecule Analyzer (MOMA) Mass Spectrometer: End-to-End Testing, Performance, and Integrated Operations Demonstration; Ryan M. Danell¹; ²Andrej Grubisic; Desmond Kaplan¹; Friso H.W. Van Amerom¹; ³Xiang Li²; ⁴Marco E Castillo; Caroline Freissinet¹; Arnaud Buch⁶; Melissa Guzman⁷; Fabien Stapleton⁷; Noel Grand⁷; Cyril Szopa¹⁰; Walter Goetz¹¹; Stephanie A. Gety¹¹; François Raulin⁶; William B. Brinckerhoff¹¹; Fred Goesmann¹¹; ¹NASA Goddard Space Flight Center, Greenbelt, MD; ²Danell Consulting, Inc., Winterville, NC; ³KapScience LLC, TEWKSBURY, MA; ⁴Mini-Mass Consulting, Inc., Hyattsville, MD; ⁵University of Maryland Baltimore County, Baltimore, MD; ⁶ATA Aerospace, Greenbelt, MD; ⁷LATMOS/IPSLS University of Versailles-Saint-Quentin-en-Yvelines, Guyancourt, France; ⁸CentraleSupélec, Paris, France; ⁹LISA, U. Paris-Est, Créteil, U. Paris Diderot, Paris, France; ¹⁰Institut Universitaire de France, Paris, France; ¹¹Max-Planck-Institut für Sonnensystemforschung, Göttingen, Germany</td>
<td>TOA pm 04:01</td>
<td>³University of Arizona, Tucson, AZ 85721</td>
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### TOB pm: Lipidomics: Targeted and Untargeted

**Chair:** Michelle Reid (ETH Zurich)

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<td>02:30</td>
<td>LipidXplorer 2.0 Web: Online tool for simplified and streamlined lipid identification, visualization and quantification by shotgun lipidomics; Eduardo Jacobo Miranda Ackerman¹; Nils Hoffmann²; Oskar Knittelfelder³; Kai Schuhmann⁴; Olga Vvedenskaya⁵; Andrej Shevchenko⁵; ¹Max Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG), Dresden, Germany; ²Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany</td>
<td>TOB pm 02:30</td>
<td>³University of Illinois at Chicago, Chicago, IL</td>
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<td>02:50</td>
<td>A Lipid Pipeline for Mapping Lipid Transducers of Exercise in Rats; David Gaul¹; Sam Moore¹; Alexandra Coomes²; Karyn A. Esser²; Brent G. Alberston²; Michael F. Hirshman³; Laure J. Goodyear⁴; Facundo M. Fernandez⁴; ¹Georgia Institute of Technology, Atlanta, GA; ²University of Florida, Gainesville, FL; ³Harvard Medical School, Boston, MA</td>
<td>TOB pm 02:50</td>
<td>³University of Illinois at Chicago, Chicago, IL</td>
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<td>Lipidomic analysis of an SCD inhibitor that reduces α-synuclein neurotoxicity; Xiaoping L Hronowski¹; Stanley Goldstein¹; Junmin Wang¹; Ru Weil¹; Andreas Weihs¹; Silke Nuber¹; Dennis Selkoe²; ²Biogen, Inc., Cambridge, Massachusetts; ³Brigham and Women’s Hospital, Harvard Medical School, Boston, Massachusetts</td>
<td>TOB pm 03:10</td>
<td>³University of Illinois at Chicago, Chicago, IL</td>
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<td>03:30</td>
<td>Mass spectrometry analysis reveals altered fatty acid levels in the brain of the symptomatic Niemann-Pick, type C1 mouse model; Melissa R. Pergande¹; Koralee C. Pathmasiri¹; Thu T.A. Nguyen¹; Stephanie M. Cologna¹; ¹University of Illinois at Chicago, Chicago, IL</td>
<td>TOB pm 03:30</td>
<td>³University of Illinois at Chicago, Chicago, IL</td>
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<td>03:50</td>
<td>Broad Lipid Coverage and Cellular-Level MALDI-Imaging of Lipids Using Oversampling Combined with Laser Post-Ionization; Shane R. Ellis¹; Andrew P. Bowman²; Jeroen F. J. Bogie³; Jerome J. A. Hendriks³; ¹Mansour Haidar²; Mikhail Belov²; Ron M.A. Heeren³; ²Molecular Horizons and School of Chemistry and Molecular Bioscience, University of Wollongong, Wollongong, Australia; ³Maastricht MultiModal Molecular Imaging (M4I) Institute, Maastricht University, Maastricht, Limburg, Netherlands, Maastricht, Netherlands; ⁴University of Arizona, Tucson, AZ 85721</td>
<td>TOB pm 03:50</td>
<td>³University of Illinois at Chicago, Chicago, IL</td>
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TOC pm 02:30 Linking Brain Tissue Lipid Distributions and Serum Biomarkers of Traumatic Brain Injury; Eric C. Gier1; Clint M. Alfaro1; Alexis N. Pulliam2; David A. Gaul1; Samuel G. Moore1; Michelle C. Laplaca1; Facundo M. Fernandez1; 1School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, 30332; 2Wallace H. Coulter Department of Biomedical Engineering, Georgia Institute of Technology, Atlanta, Georgia

TOC pm 02:50 Profiling RNA Modifications in Central Nervous Tissue by Mass Spectrometry Reveals Spatiotemporal Heterogeneity in the Neural Epitranscriptome during Non-Associative Learning; Kevin Clark1; Yanqi Tan2; Jonathan V Sweedler1,4; 1Beckman Institute, Urbana, IL; 2University of Illinois at Urbana-Champaign, Urbana, IL

TOC pm 03:10 Cell and Proteoform-Specific Top-Down Proteomics Reveals Biomarkers of Acute Liver Rejection; Paul M Thomas1; Robert V Gerbasi1; Rafael D Melani1; Ryan T Fellers1; Joseph B Green1; Richard D Leduc1; Timothy K. Toby1; Joshua Levitsky2; Neil L Kelleher3; 1Northwestern University, Evanston, IL; 2Northwestern University, Chicago, IL

TOC pm 03:30 Spatially-Targeted Proteomics for Analysis of Host-Pathogen Interactions in Staphylococcus aureus; Emma R Guiberson1,2; Daniel J Ryan1,2; Andy Weiss3; Eric P Skaar3; Richard M. Caprioli1,2,4,5,6; Jeffrey M. Spragins1,2,4; 1Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN 37205; 2Department of Chemistry, Vanderbilt University, Nashville, TN; 3Department of Pathology, Microbiology and Immunology, School of Medicine, Vanderbilt University, and Vanderbilt University Medical Center, Nashville, TN; 4Department of Biochemistry, Vanderbilt University, Nashville, TN; 5Department of Medicine, Vanderbilt University, Nashville, TN; 6Department of Pharmacology, Vanderbilt University, Nashville, TN

TOC pm 03:50 Equine Biological Passport using Orbitrap Exploris 480; Sophie Bromilow1; Claudia P.B. Martins2; Amanda Lee3; Michael W. Senko4; Scott D Stanley1; 1University of Kentucky, Lexington, KY; 2ThermoFisher Scientific, San Jose, CA

TOC pm 04:10 Targeted and Untargeted Metabolomics for Monitoring and Assessing Soldier Tactical Readiness and Effectiveness; Elizabeth S Dhummakupt1; Richard Lawrence1; Ethan McBride1; Phillip Mach1; Conor Jenkins2; Trevor Glaros1; Erika Hussey1; John Ramsay3; 1CCDC-Chemical Biological Center, APG-EA, MD; 2Excet, Inc., Springfield, VA; 3CCDC-Soldier Center, Natick, MA

TOD pm 04:10 Ambient mass spectrometry imaging of biological tissue with atmospheric pressure UV-laser desorption low temperature plasma post-ionization; Bin Yan1; Rory T Steven1; Teresa Murtia2; Efstatios A Elia1; Marcel Niehaus1; Kenneth N Robinson1; Martin Metodiev1,2; Josephine Bunch1,2; 1National Physical Laboratory, Teddington, United Kingdom; 2Imperial College London, London, United Kingdom
TOF pm: Cannabis Testing
Chair: Brigitte Simons (Pasha Brands)

TOE pm 02:30 Cannabinoidomics – An Analytical Tool to Understand the Effect of Medical Cannabis Treatment in Clinical and Preclinical Studies; Paula Berman1; Liron Sulimani2; Anat Gelfand1; Keren Amsalem1; Gil M Lewitus1; David Mein1; 1Technion - Israel Institute of Technology, Haifa, Israel; 2Cannasoul Analytics, Caesarea, Israel

TOE pm 02:50 Investigation of Tetrahydrocannabinol (Δ9-THC) and Cannabidiol (CBD) in Smoke by Application of an On-Line Photo Ionization Mass Spectrometry; Sven Ehler1, 2; Jan Heide2; Andreas Walte1; Ralf Zimmermann2, 3; 1Photonion GmbH, Schwerin, Germany; 2University of Rostock, Institute of Chemistry, Division of Analytical and Technical Chemistry, Rostock, Germany; 3Helmholtz Center, Munich, Germany

TOE pm 03:10 Vaping-Related Outbreak: Unique Information from Direct Analysis in Real-Time Mass Spectrometry; Travis M. Falconer1; Adam C. Lanzarotta1; Robert A. Wilson1; Rick A. Flurer1; 1US Food & Drug Administration, Cincinnati, OH

TOE pm 03:30 Characterizing Products Intended for Inhalation After High-Temperature Vaporization; Nahanni Sagar1; Seamus Riordan-Short1; Rob O’Brien1, 2; Matthew Noestheden1, 2; 1Supra R&D, Kelowna, BC; 2University of British Columbia, Kelowna, BC

TOE pm 03:50 Characterization of Beverage Products containing Cannabidiol (CBD) by GC-MS and GCxGC-MS; Elizabeth Humston-Fulmer1; Christina Kelly1; David E Alonso1; Joe Binkley1; Lorne Fell1; 1LECO Corporation, Saint Joseph, MI

TOE pm 04:10 A Robust LC-QQQ Method for the Analysis of Pesticides and Mycotoxins in Cannabis Samples According to Health Canada Regulations; Hanieh Peyman1; Heather Gamble1; Kaveh Kahan1; 1Sigma Analytical, Scarborough, ON

TOF pm: Nucleic Acids and Oligonucleotides
Chair: Amber Mosley (Indiana University)

TOF pm 02:30 Revealing molecular detail of DNA triplexes to underpin antigene technology; Alexander Begbie1; Jack Klose1; Jiawei Li1; Tara L Pukala1; 1University of Adelaide, Adelaide, Australia

TOF pm 02:50 Ribonucleic Acid Sequence Characterization by Activated Ion-Negative Electron Transfer Dissociation (AI-NETD) Mass Spectrometry; Trenton M Peters-Clarke1; Qiuwen Quan1; Dain R Brademan1; Alexander S Hebert1; Michael S Westphall1; Joshua J Coon1; 1University of Wisconsin-Madison, Madison, WI

TOF pm 03:10 Hybridization LC-MS/MS: An Alternative Bioanalytical Method for Anti-Sense Oligonucleotide Quantitation in Plasma and Tissue Samples; Pei Li1; Yuqing Gong1; Jaeeah Kim2; Jp Gilbert1; Hannah Certo1; Rachel Groth1; Michael Rooney1; 1Biogen, Cambridge, MA; 2Atrium Staffing, Boston, MA

TOF pm 03:30 Database Search of Tandem Mass Spectra of Oligonucleotides; Marshall W. Bern1; Rose D Lawler1; Wilfred Tang1; Eric Carlson1; Maria Basanta-Sanchez2; Ines C Santos3; Jennifer S Brodbelt4; 1Protein Metrics Inc., Cupertino, CA; 2University of Texas at Austin, Austin, TX

TOF pm 03:50 Novel aspects of augmenting protein–nucleic acid cross-link identification by high-field asymmetric-waveform ion-mobility mass spectrometry (FAIMS); Alexander Wulf1; Rosa Viner2; Timo Sachsenberg2; Oliver Kohlbacher2; Henning Urlaub3, 4, 5; 1Max Planck Institute for biophysical chemistry, Göttingen, Germany; 2Thermo Fisher Scientific, San Jose, CA; 3Center for Bioinformatics, University of Thübingen, Thübingen, Germany; 4Max Planck Institute for biophysical chemistry, Göttingen, Germany; 5Bioanalytics Group, University Medical Center Göttingen (UMG), Göttingen, Germany

TOF pm 04:10 On-line capillary electrophoresis-UVPD-mass spectrometry for the characterization of nucleic acids; Ines C Santos1; Jada N. Walker1; Marshall Bern2; Maria Basanta-Sanchez2; Jennifer S Brodbelt4; 1University of Texas at Austin, Austin, TX; 2Protein Metrics Inc., Cupertino, CA
TOG pm: Glycopeptides and Glycoproteins
Chair: Lingjun Li (University of Wisconsin)

TOG pm 02:30 Effective MS-Based Chemical Methods for Comprehensive Analysis of Glycoproteins; Ronghu Wu¹; Fangxu Sun¹; ¹Georgia Institute of Technology, Atlanta, GA

TOG pm 02:50 Enhanced N-sialoglycoproteomic Profile by Using Zwitter-Ionic Hydrophilic Interaction Chromatography (ZIC-HILIC); Yi-Ju Chen¹; Ta-Chi Yen¹; Yu-Hsien Lin¹; Kai-Hooi Khoo²; Yu-Ju Chen¹; ¹Institute of Chemistry, Academia Sinica, Taipei, Taiwan; ²Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan

TOG pm 03:10 Comprehensive N- and O-Glycoproteomics with MSFragger Mass Offset Search; Daniel A. Polasky¹; Fengchao Yu¹; Guo Ci Teo¹; Felipe da Veiga Leprevost¹; Alexey I. Nesvizhskii¹; ¹University of Michigan, Ann Arbor, MI

TOG pm 03:30 Multi-Glycomic Platform for Mapping the Human Brain Glycocalyx in Alzheimer’s Disease Patients in a Region-Specific Manner using nanoLC-MS Methods; Jennyfer Tena¹; Mariana Barboza¹; Maurice Wong¹; Carlito B Lebrilla¹; ¹UC Davis, Davis, CA

TOG pm 03:50 How unique is our plasma proteome? Answers from top-down native mass spectrometry; Albert J.R. Heck; Utrecht University, Utrecht, Netherlands

TOG pm 04:10 Multiplexed Imaging Mass Spectrometry of the Extracellular Matrisome using Serial Enzyme Digests from Formalin-Fixed Paraffin Embedded Tissue Sections; Cassandra L Clift¹; Anand Mehta¹; Peggi M Angel¹; ¹Medical University of South Carolina, Charleston, SC

TOH pm: Fundamentals: Native MS
Chair: Saiful Chowdhury (University of Texas at Arlington)

TOH pm 02:30 Design and application of an alpha particle electrospray source for native mass spectrometry analysis of theoretically unresolvable glycoprotein therapeutic targets; Elizabeth Hecht¹; Ben Aguilar²; Ananya Dubey²; Wendy Sandoval¹; Henry Benner²; ¹Genentech Inc., South San Francisco, CA; ²Ion Dx, Monterey, CA

TOH pm 02:50 Statistical Analysis of Ultraviolet Photodissociation of Native-Like Proteins; Luis A Macias¹; Jennifer Brodbelt¹; ¹University of Texas at Austin, Austin, TX

TOH pm 03:10 Trends and applications from >10,000 fragment ions produced by higher-energy collisional dissociation of 159 native monomers and 70 native complexes; Ashley N Ives¹; Taojunteng Su¹; Kenneth R Durbin¹; Bryan P Early¹; Henrique dos Santos Seckler¹; Ryan T Fellers¹; Richard D Leduc¹; Luis F Schachner¹; Steve M Patrie¹; Neil L Kelleher¹; ¹Northwestern University, Evanston, IL/60208; ²Proteinaceous, Evanston, IL

TOH pm 03:30 Combining native mass spectrometry with mass photometry to quantify ultra-heterogeneous protein assemblies; Miranda P Collier¹; Dominik Saman¹; Justin LP Benesch¹; ¹University of Oxford, Oxford, United Kingdom

TOH pm 03:50 Electrospray Surface Charge Describes Protein Molecular Motion; Rod Chalk¹; Oktawia Borokowska¹; Petra Born³; Ole Tietz¹; Opher Gileadi¹; Nicola Burgess-Brown¹; ¹Oxford University, Oxford, United Kingdom; ²Lanza, Slough, United Kingdom; ³Max Plank Institute, Dresden, Germany

TOH pm 04:10 Improving mass measurements of protein complexes through IR activation coupled with charge reduction ion/ion reactions; Kenneth W. Lee¹; Christopher P. Harrilal¹; Liangxuan Fu¹; Gregory S. Eakins¹; Scott A. McLuckey¹; ¹Purdue University, West Lafayette, IN
WEDNESDAY AM ORALS

WOA am: Instrumentation: Innovative Separations Approaches Coupled to MS
Chair: Honglan Shi (Missouri University)

WOA am 08:30  Qualitative and quantitative advantages of Liquid Electron Ionization (LEI) interface in pesticides analysis of complex matrices; Veronica Termopolii1; Giorgio Famigli1; Pierangela Palma1,2; Mansoor Saeed1; Simon J. Perry1; Pablo Navarro3; Helene Fain1; Achille Cappiello1,2; 1University of Urbino, Urbino, Italy; 2Vancouver Island University, Nanaimo, BC; 3SYNGENTA, Bracknell, United Kingdom

WOA am 08:50  New Double Barrel ESI Source and Novel Tandem NanoLC-MS Setup Enables 24/7 Proteome Profiling and Close to 100% MS Utilization; Runsheng Zheng1; Thomas Lanzinner2; Georg Völkle3; Christopher Pynn1; Jan Linnemann1; John Modrow2; Wim Decrop3; Andreas Tebbe2; Peter Jehle1; Oleksandr Boychenko4; 1Thermo Fisher Scientific, Germering, Germany; 2Evotec (München) GmbH, Martinsried, Germany; 3Sonation GmbH, Biberach, Germany; 4Thermo Fisher Scientific, Germering, Germany

WOA am 09:10  Native Ion-Mobility Coupled to a Q Exactive UHMR Orbitrap MS: Protein Complexes at Ultra High Resolution; Jacob W. McCabe1; Christopher S. Mallis1; Claudia I. Kocurek1; Joanna K. Denton1; John M. Gordon1; Mehdi Shirzadeh1; Michael L. Pottash1; Arthur Laganowsky1; David H. Russell1; 1Texas A&M University, College Station, TX

WOA am 09:30  A Liquid-phase Ion Trap for Ion Trapping, Transfer and Sequential Ejection in Solutions; Jie Hong; Beijing Institute of Technology, Beijing, China

WOA am 09:50  A Novel Nanoflow ESI Probe Optimized for Emitters with Chromatographic Packing; Yang Kang1; Leigh Bedford1; Stanislav Potryala1; Bradley B. Schneider1; 1SCIEX, Concord, ON

WOA am 10:10  Towards Online Single Cellular Metabolomics from a Cell Suspension Using Electrospray; Catherine Munetanu1, Shahd Abuhelal1, Chelsea Nikula1, Daniel Simon1, David Gaboriau1, Andreas Dannhomm2, Efstatios Elias2, Richard Goodwin2, Josephine Bunch2, 4, Zoltan Takats1; 1Imperial College London, London, United Kingdom; 2National Physical Laboratory, Teddington, United Kingdom; 3AstraZeneca, BioPharmaceuticals R&D, Imaging and AI, Clinical Pharmacology and Safety Sciences, Cambridge, United Kingdom; 4Imperial College London, London, United Kingdom

WOB am: Cancer Research
Chair: Jurre Kamphorst (Rheos Medicines Inc.)

WOB am 08:30  Quantitative Proteomics of the Cancer Cell Line Encyclopedia; David Nusinow1; John Szypf2; Steven P Gyi2; 1Harvard Medical School, Boston, MA; 2Harvard Medical School, Boston, MA

WOB am 08:50  Multi-omic discovery of metabolic rewiring in triple-negative breast cancer following mitochondrial folate transport ablation; Qiuying Chen1; Joshua B. Zuk1; Christine A. Miller2; Steve M. Fischer2; Steven S. Gross1; 1Weill Cornell Medicine, New York, NY; 2Agilent Technologies, Santa Clara, CA

WOB am 09:10  Mass Spectrometry Imaging of N-Glycan Profiles in Tissue Microarrays of Metastatic Breast Cancer Patients Reveals Glycosylation Patterns in Metastasis; Klara Scupakova1; Oluwatobi Adelaja2; Benjamin Balluff1; Caitlin M. Tressler1; Pedram Argani2; Ron M.A Heeren1; Kristine Glunde1, 2; 1DKFZ, Heidelberg, Germany; 2Max Planck Institute for Immunobiology and Epigenetics, Freiburg, Germany

WOB am 09:30  Recombinant MHC class I protein with isotope coded peptides enables relative and absolute quantification of the immunopeptide; Lauren E Stopfer1, 2; Joshua M Mesfin2; Brian A Joughin1, 2; Douglas A Lauffenburger1, 2; Forest M White1, 2; 1Koch Institute for Integrative Cancer Research, Cambridge, MA; 2Department of Biological Engineering, Massachusetts Institute of Technology, Cambridge, MA

WOB am 09:50  Streamlined Proteomic Profiling of quantity-limited Clinical Tissue facilitated by automated Sample Preparation and Mass Spectrometry; Torsten Mueller1; Mathias Kalidof1, 2; Romano Hebler2; Scarlet Koch3; Marcel Kool1, 4; Kristian Pagler1, 4; Jeroen Krijgsveeld1; 1DKFZ, Heidelberg, Germany; 2EMBL - European Molecular Biology Laboratory, Heidelberg, Germany; 3Buerk Daltonics, Bremen, Germany; 4KiiT - Hopp Children's Cancer Center, Heidelberg, Germany

WOB am 10:10  Determining the Origins of Fumarate Accumulation in Patient-Derived Fumarate-Deficient Tumor Cell Lines; Daniel Crooks1; Nunziata Maio2; Ye Yang3; Youfeng Yang3; Bhargav Arimilli3; Ramon Sun4; Tracey Rouault5; Richard Higashi5; Teresa Fan5; Andrew Lane5; W. Marston Linehan1; Penghui Lin4; 1National Cancer Institute, Bethesda, MD; 2Eunice Kennedy Shriver NICHD, National Institutes of Health, Bethesda, Maryland; 3UT Southwestern Medical Center, Dallas, TX; 4University of Kentucky, Lexington, KY
WOC am: Drug Target Identification by MS
Chair: Silvi Chacko (Bristol-Myers Squibb)

WOC am 08:30 Automated data analysis workflow for high throughput compound screening using Bruker MALDI-TOF platform; Serhiy Hnatyshyn1; Jingjing Deng1; Joseph Scaletta2; Rostyslav Hnatyshyn3; David Harden1; 1BMS Co., Princeton, NJ; 2Rowan University, Glassboro, NJ 08028

WOC am 08:50 Label-free target identification in one-pot 2D format: evaluation and method comparison using a broad-spectrum kinase inhibitor; Yingrong Xu1; Graham M. West1; Mario Abdelmessih1; Robert A. Everley1; 1Pfizer Worldwide Research and Development, Groton, CT

WOC am 09:10 Kinase specificity characterization of a PROTAC directed against BRAFV600E; Ganna Posternak1, 2; Xiaojing Tang1; Pierre Monsienneuv1; Ting Jin2; Hugo Lavoie1; Zhe Yin3, 4; Ahmed Aman1; Michael Prakesch2; Gennady Podu2; Alexandre Cassandre3; Stefan Maier1; Julia Kitaygorodsky1, 4; Lars Albrechtsen2; Karen Colwill1; Robert Batey1; Milko Taipale1, 5; Igor Kourinov1; David Uehling3; Anne-Claude Gingras1, 4; Rima Al-Awar2; Marc Therrien3; Frank Sicheri1, 4; 1Lunenfeld-Tanenbaum Research Institute at Mount Sinai Hospital, Toronto; 2Ontario Institute for Cancer Research, Toronto, ON; 3University of Montreal, Montreal, QC; 4University of Ottawa, Ottawa, ON; 5Donnelly Centre for Cellular and Biomolecular Research, Toronto, ON; 6NE-CAT, Argonne, IL

WOC am 09:30 Quantitative proteomics identifies novel substrates of pomalidomide; Raghothama Chaerkady1; Saghar Nourian1; Hsiang-En Hsu1; Nazzareno Dimasi1; Sonja Hess1; 1AstraZeneca R&D, Gaithersburg, MD

WOC am 09:50 An Integrative Genomics, Metabolomics and Lipidomics Approach to Identify and Validate New Pharmaceutical Drug Targets; Silvia Aldi1; Gregory Hamm2; Lubjica Matic3; Danielle Van Keulen3; Dennie Tempel4; Kim Holmstrom5; Boye Schnack5; Valur Emilsson6; Mariette Lengquist7; Per Eriksson7; David Bonne8; Alain J Gool9; Jonathan Stauberg6; Ulf Hedlin2; Eva Hurt Camejo10; 1Karolinska Institute, Solna, Sweden; 2ImaBiotech, Loos, France; 3IRCCS - Istituto di Ricerche Farmacologiche "Mario Negri", Milan, Italy; 4CardioGenx, Rotterdam, Netherlands; 5Bioneer, Horsholm, Denmark; 6Icelandic Heart Association, Kopavogur, Iceland; 7TNO, Zeist, Netherlands; 8ImaBiotech, Billerica, Massachusetts; 9AstraZeneca R&D, Gothenburg, Sweden

WOC am 10:10 Simultaneous detection of protein target engagement and functional readout for in-depth characterization of targeted protein degraders; Alexey L Chernobrovkin1; Daniele Amadio1; Cindy Caceres Körner1; Tomas Friman1; Johan Lengqvist1; Isabel Martin Caballero1; Daniel Martinez Molina1; 1Pelago Bioscience AB, Solna, Sweden

WOC am: Informatics: Data-Independent Acquisition
Chair: Brian Searle (Institute for Systems Biology)

WOC am 08:30 Strategies to improve reproducibility of large-scale data-independent acquisition mass spectrometry measurements acquired on multiple instruments over an extended period; Rebecca C Poulos1, 2; Peter G Hains1; Rohan Shah1; Natasha Lucas1; Dylan Xavier1; Sríkanth S Manda1; Asim Anees1; Jennifer MS Koh1; Sadia Mahboob1; Max Wittman1; Steven G Williams1; Erin K Sykes1; Michael Hecker1; Michael Dausmann1; Merridee A Wouters1; Keith Ashman2; Jean Yang3; Peter Wild4, 5; Anna Defazio6, 7, 8; Rosemary Ballesne1; Brett Tully1; Ruedi Aebersold1, 9; Ljubica Matic10; Terence P Speed11, 12; Yansheng Lui13, 14; Roger R Redel1; Philip J Robinson1; Qing Zhong1; 1Children’s Medical Research Institute, Faculty of Medicine and Health, The University of Sydney, Westmead, Australia; 2Sciex, 2 Gilda Court, Mulgrave, Australia; 3School of Mathematics and Statistics, The University of Sydney, Sydney, Australia; 4Dr. Senckenberg Institute of Pathology, University Hospital Frankfurt, Frankfurt am Main, Germany; 5Department of Pathology and Molecular Pathology, University Hospital Zurich, Zurich, Switzerland; 6Centre for Cancer Research, Westmead Institute for Medical Research, Westmead, Australia; 7Faculty of Medicine and Health, The University of Sydney, Westmead, Australia; 8Department of Gynaecological Oncology, Westmead Hospital, Westmead, Australia; 9Department of Biology, Institute of Molecular Systems Biology, ETH Zürich, Zurich, Switzerland; 10Faculty of Science, University of Zürich, Zurich, Switzerland; 11Bioinformatics Division, Walter and Eliza Hall Institute of Medical Research, Parkville, Australia; 12Department of Mathematics and Statistics, University of Melbourne, Melbourne, Australia; 13Department of Pharmacology, Yale University School of Medicine, New Haven, CT; 14Yale Cancer Biology Institute, Yale University, West Haven, CT

WOC am 08:50 Deep learning enables automated and extensible peak group identification for multi-technology chromatogram-based data-independent acquisition data analysis; Leon L Xu1, 2, 3; Hannes L Rööst1, 2, 3; 1University of Toronto, Toronto, ON; 2Department of Molecular Genetics, University of Toronto, Toronto, ON; 3The Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON

WOC am 09:05 Multidimensional data extraction from scanning quadrupole SWATH data; Gordana Ivosev1; Nic Bloomfield1; Stephen Tate2; 1SCIEX, Concord, ON; 2SCIEX, Concord, Ontario

WOC am 09:30 Skyline integrates the Prosit server protocol for proteome-wide DIA data analysis using on-demand fragment intensity and iRT prediction; Tobias Rohde1; Tobias Schmidt2; Nicholas Shulman1; Johannes Rank2; Bernhard Kuster2; Michael J MacCoss3; Mathias Wilhelm5; Brendan Maclean1; 1Univ of Washington,
### WOF am 09:50

**Removing the hidden data dependency of DIA with predicted spectral libraries:** Bart Van Puyvelde¹,²; Sander Willems¹,²; Ralf Gabriels³,⁴; Simon Daclerk¹,²; Laura De Clerck¹,²; Sofie Vande Casteele¹,²; An Staes⁵; Francis Impens¹; Dieter Deforce¹,²; Lennart Martens¹; Sven Degroeve¹; Maarten Dhaenens¹,²; ¹Ghent University, Faculty of Pharmaceutical Sciences, Ghent, Belgium; ²ProGenTomics, Ghent, Belgium; ³Ghent University, Ghent, Belgium; ⁴VIB - UGent Center for Medical Biotechnology, Gent, Belgium; ⁵VIB - Department of Medical Protein Research, Ghent, Belgium

### WOF am 10:10

**End-to-End Phenotype Prediction using Data Independent Acquisition Mass Spectrometry Tensor:** Fangfei Zhang¹; Shaoyang Yu²; Lirong Wu²; Zelin Zang¹; Yaoting Sun¹; Yi Xiao¹; Ziqing Li³; Zhongzhi Luan³; Tiannan Guo⁴; Westlake University, Hangzhou, China; ²Westlake University, Hangzhou, China; ³Beihang University, Beijing, China

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**WOE am: GC/MS, GCxGC/MS, GC-MS/MS, and GC/HRMS**

Chair: Hannah Libratore (U.S. Environmental Protection Agency)

### WOE am 08:30

**Finding Needles in a Haystack: Pesticide Analysis in Hemp with GCxGC and High Resolution Mass Spectrometry:** Todd Richards¹; Joe Binkley²; Christina Kelly²; ¹LECO, St. Joseph, MI; ²LECO Corporation, Saint Joseph, MI

### WOE am 08:50

**Cannabinoids Analysis by GC-MS with Cold EI:** Aviv Amirav¹,²; Alexander B. Fialkov³; Tal Alon²,³; Ksenia Margolin-Eren³; Benjamin Neumark³; ¹Tel-Aviv University, Tel-Aviv, Israel; ²Aviv Analytical, Hod Hasharon, Israel; ³Tel Aviv University, Tel Aviv, Israel

### WOE am 09:10

**Bio-oil's isomeric compositions and their reactivity revealed by gas chromatography coupled to Fourier transform ion cyclotron resonance mass spectrometry:** Diana Catalina Palacio Lozano¹; Hugh E. Jones¹; Remy Gavard¹; Mary J. Thomas¹; Claudia X. Ramirez²; Christopher A. Wootton¹; Jose Aristobulo Chaparro¹; Peter B O'Connor¹; Simon E. F. Spencer¹; David Rossell²; Enrique Mejia Ospino²; Matthias Witt³; Mark P. Barrow¹; ¹University of Warwick, Coventry, United Kingdom; ²University Industrial de Santander, Santander, Colombia; ³Instituto Colombiano del Petroleo (ICP-Ecopetrol), Piedecuesta, Colombia, Colombia; ¹Universitat Pompeu Fabra, Barcelona, Spain; ²Bruker, Bremen, Germany

### WOE am 09:30

**Non-targeted detection of fluorinated compounds using dielectric barrier discharge nano-electrospray ionization:** Kunyu Zheng¹; Joseph E. Lesniewski¹; Michael J. Dolan Jr¹; Wanqing Li¹; Tyler Metallo¹; Kaveh Jorabchi¹; ¹Georgetown University, Washington, DC

### WOE am 09:50

**Delivering quality data in breath biomarker discovery by TD-GCxGC-TOF MS:** Laura McGregor¹; Nick Bukowski¹; Pete Grosshans¹; Bob Green¹; Anthony Buchanan¹; David Bowman¹; ¹SepSolve Analytical, Peterborough, United Kingdom; ²SepSolve Analytical, Waterloo, ON

### WOE am 10:10

**Lend Me Your Ears: Two-Dimensional Gas Chromatography-Mass Spectrometric Analysis of Earwax for Disease Diagnosis:** Rabi A Musah¹; Allix M. Coon¹; John Dane²; Robert B Cody²; ¹University at Albany - SUNY, Albany, NY; ²JEOL USA, Inc., Peabody, MA

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**WOF am: Top Down Protein Analysis**

Chair: Laura Herring (UNC-Chapel Hill)

### WOF am 08:30

**A Quantitative Atlas of the Histone Proteoforms of the Brain and Applications to Disease:** Tao Wang¹; Matthew V. Holt¹; Nikit Venishetty²; Nicholas L. Young¹; ¹Baylor College of Medicine, Houston, TX; ²Rice University, Houston, TX

### WOF am 08:50

**Characterizing Large Heart Proteoforms (Up to 223 kDa) by Novel Top-down Proteomic Strategy:** Trisha Tucholski¹; Kyle A. Brown¹; Jake A. Melby¹; Ying Ge¹; ¹University of Wisconsin-Madison, Madison, WI

### WOF am 09:10

**FLASHDeconv: ultrafast high-quality deconvolution for top-down MS1/MS2 spectra:** Kyowon Jeong¹; Maša Babović²; Jihyung Kim¹; Pavel V Shihaia³; Sebastian Gibb³; Ole N Jensen³; Oliver Kohlbacher¹,⁴,⁵; ¹University of Tübingen, Tübingen, Germany; ²University of Southern Denmark, Odense, Denmark; ³University Medicine Greifswald, Greifswald, Germany; ⁴Max Planck Institute for Developmental Biology, Tübingen, Germany; ⁵University Hospital Tübingen, Tübingen, Germany

### WOF am 09:30

**Application of cylindrical FAIMS for top-down identification of proteins directly from bacterial colonies by LESA MS:** Jana Havlikova¹; Robin C. May¹; Iain B. Styles¹; Helen J. Cooper¹; ¹University of Birmingham, Birmingham, United Kingdom
WOH am 09:50  **Predicting electrophoretic mobility of proteoforms for large-scale top-down proteomics;** Daoyang Chen\(^1\); Rachele Luebckyj\(^1\); Zhichang Yang\(^1\); Elijah Mccool\(^1\); Xiaoqing Shen\(^1\); Qianjie Wang\(^1\); Tian Xu\(^1\); Liangliang Sun\(^1\); \(^1\)Michigan State University, East Lansing, MI

WOH am 10:10  **Denatured/Native Capillary Electrophoresis and Top-Down Proteomics for In-depth Proteoform Characterization;** Kevin Joos\(^1\); Rafael D Melani\(^1\); Luis F Schachner\(^1\); Nicholas W Bateman\(^2\); Thomas P Conrads\(^2\); 3; Paul M Thomas\(^1\); Philip D Compton\(^1\); Neil L Kelleher\(^1\); 1Northwestern University, Evanston, IL/60208; 2Women’s Health Integrated Research Center at Inova Health System, Annandale, VA/22033; 3Women’s Service Line, Inova Health System, Falls Church, VA/22042

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<tr>
<td>WOG am 08:30</td>
<td>More than QuEChERS is the QuEChERSER Mega-Method for Analysis of Pesticides, Veterinary Drugs, and Other Contaminants in Foods; Steven J Lehotay; USDA ARS, Wyndmoor, PA</td>
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<td>WOG am 08:50</td>
<td>Significant improvements to the LC/MRM-based detection of herbicides using iTTrEnDi; Christian A Rosales(^1); Samuel W Shields(^2); Chelsey Aulenback(^1); Krysten Sheedy(^1); Karl V Wasslen(^1); Erdim Sertoglu(^3); Kym Faull(^1); Jeffrey M Manthorpe(^1); Jeffrey C Smith(^1); 1Carleton University, Ottawa, ON; 2University of Texas Austin, Austin, TX; 3University of California, Los Angeles, Los Angeles, CA</td>
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<td>WOG am 09:10</td>
<td>A 3D Mass Spectrometry-based Method for the de Novo Structural Elucidation of Polysaccharides; Juan J Castillo(^1); Ace G. Galermo(^2); Matthew J. Amicucci(^2); Eshani Nantida(^1); Ye Chen(^1); Carlito B Lebrilla(^2); 1University of California, Davis, Davis, CA; 2University of California Davis, Davis</td>
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<td>WOG am 09:30</td>
<td>Development of a standard quality assurance control mixture for evaluating non-targeted liquid chromatography/high resolution mass spectrometry (LC/HR-MS) method performance; Christine Fisher(^1); Jacob H. Premo(^1); Ann M. Knollhoff(^1); 1FDA, College Park, MD</td>
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<td>WOG am 09:50</td>
<td>Evaluation of the segmented non-target data acquisition (SWATH/vDIA) in QToF and QOrbitrap for pesticide residue analysis; Łukasz Rajski(^1); Iciar Beraza(^1); María José Gómez Ramos(^1); Amadeo R. Fernández-Alba(^1); European Union Reference Laboratory for Pesticide Residues in Fruit &amp; Vegetables. University of Almería, Agrifood Campus of International Excellence (ceiA3), Almería, Spain</td>
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<td>WOG am 10:10</td>
<td>Determination of Decomposition in Seafood Products by High-Resolution Mass Spectrometry with Sensory-Driven Modeling; Randy Self(^1); Michael G. McLendon(^1); Christopher M. Lock(^1); 1U.S. FDA, Bothell, WA</td>
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<td>WOH am 08:30</td>
<td>Revisiting the Yen-Mullins Model of Petroleum Asphaltenes; Ryan P Rodgers(^1); Martha L Chacón-Patirío(^1); Sydney F Niles(^2); Alan G Marshall(^1); 1National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; 2Florida State University, Tallahassee, FL</td>
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<td>WOH am 08:50</td>
<td>Novel four dimensional approach for the structural characterization of neutral nitrogen compounds using UHPLC-IM-QTOF analysis on pre-fractionated vacuum gas oils; Julie Guillemant(^1); Alexandra Berlioz-Barbier(^1); Marion Lacouve-Nègre(^1); Luis Pereira De Oliveira(^1); Jean-François Joly(^1); Ludovic Duponchel(^2); 1IFP Energies Nouvelles, Solaize, France; 2Univ. Lille, CNRS, UMR 8516 - LASIR, Lille, France</td>
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<td>WOH am 09:10</td>
<td>Comprehensive Screening of polycyclic aromatic hydrocarbon like compounds using GC-APLI-TIMS-TOF MS/GC-El-MS; Clement Alibade Olanrewaju(^1); Cesar E Ramirez(^2); Francisco A. Fernandez-Lima(^1); 1Florida International University, Miami, FL; 2Advance Mass Spectrometry Facility, Florida International University, Miami, FL 33199.</td>
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<td>WOH am 09:30</td>
<td>GC-SICRIT-HRMS for detailed analysis of saturated and unsaturated components in complex hydrocarbon mixtures; Markus Weber(^1); Jan-Christoph Wolf(^2); Christoph Haisch(^1); 1TU Munich, Munich, Germany; 2Plasmon GmbH, Augsburg, Germany</td>
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<td>WOH am 09:50</td>
<td>Biomass Comparison, Characterization, and Quantification with Analytical Pyrolysis GCxGC-MS; Brittany D.M. Hodges(^1); Amber N. Hoover(^1); Chenlin Li(^1); Gary S. Groenewold(^1); Christopher A. Zarzana(^1); Lynn M. Wendl(^1); Kyle Rigg(^1); Allison E. Ray(^1); 1Idaho National Laboratory, Idaho Falls, ID</td>
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<td>WOH am 10:10</td>
<td>High Resolution Orbitrap Mass Spectrometry Analysis of Oxygenated Hydrocarbons Found in Fresh Water Contaminated by a Crude Oil Spill; Nicole E. Heshka(^1); Kerry M. Peru(^2); John V. Headley(^2); Heather D. Dettmann(^1); 1Natural Resources Canada, CanmetENERGY, Devon, AB; 2Environment and Climate Change Canada, Saskatoon, SK</td>
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| WOA pm 02:30 | The Structures and Stabilities of Cytochrome P450 – Drug Complexes Depend upon Their Local Lipid Environments | Kristine F. Parsons¹; Katherine Gentry²; Carlo Barnaba³; Marina Sarcinella¹; Colleen M. Riordan¹; Sugyan Dixit¹,³; Sarah M Fantin¹; Varun V. Gadkari¹; Ayyalusamy Ramamoorthy²; Ryan C. Bailey¹; Brandon T Ruotolo¹;¹ Department of Chemistry, University of Michigan, Ann Arbor, Michigan;² Biophysics Program and Department of Chemistry at University of Michigan, Ann Arbor, MI;³ Department of Pharmacology, Feinberg School of Medicine, Northwestern University.  
| WOA pm 02:50 | Native Mass Spectrometry and Surface Induced Dissociation Complement Cryo-Electron Microscopy for Structural Elucidation of a Heterogeneous Pseudo-enzyme Complex | Mowei Zhou¹; Chen Du²; Zachary Vanaermann²; Irina Novikova¹; Aivett Bilbao¹; Vicki H. Wysocki²; Hanjo Hellmann³; James Evans¹,³;¹ Pacific Northwest National Laboratory, Richland, WA;² The Ohio State University, Columbus, OH;³ Washington State University, Pullman, WA  
| WOA pm 03:10 | Protein ion conformations after electrospray ionization – a study with soft-landing and electron microscopy | Jingjin Fan¹; Zi Yang²,³; Xiaoyu Zhou¹; Zheng Ouyang¹;¹ State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China;² Ministry of Education Key Laboratory of Protein Sciences, Beijing Advanced Innovation Center for Structural Biology, School of Life Sciences, Tsinghua University, Beijing, China;³ Tsinghua-Peking Joint Center for Life Sciences, Tsinghua University, Beijing, China  
| WOA pm 03:30 | An isotope depletion strategy for improved high resolution native mass spectrometry of metalloprotein complexes | Kelly J. Gallagher¹; Jennifer Ross¹; C. Logan Mackay¹; David P. A. Kilgour²; Jon Marles-Wright³; David J Clarke¹;¹ University of Edinburgh, Edinburgh, United Kingdom;² Nottingham Trent University, Nottingham, United Kingdom;³ Newcastle University, Newcastle-upon-Tyne, United Kingdom  
| WOA pm 03:50 | Lipids are very basic in the gas phase: implications for native mass spectrometry | Jesse W Wilson¹; Zachary M. Miller¹; J. Diana Zhang¹; Micah T. Donor¹; Amber D. Rolland¹; Samantha O. Shepherd¹; William A. Donald¹; James S. Prell¹;¹ University of Oregon, Eugene, OR;² University of New South Wales, Sydney, Australia  
| WOA pm 04:10 | Empty Slot. Stay tuned for promoted selection to be made. | |
| WOB pm 02:30 | Spectrum acquisition and evaluation for building the NIST tandem MS library 2020 | Yuxue Liang¹; Pedatsur Neta¹; Xiaoyu Yang¹; Stephen E. Stein¹; National Institute of Standards and Technology, Gaithersburg, MD  
| WOB pm 02:50 | Fast, Flexible and Feature-Rich Computation of Peptide and Proteoform Posterior Error Probabilities Using Binary Decision Trees in MetaMorpheus | Michael R. Shortreed¹; Lei Lu¹; Robert J. Millikin¹; Rachel M. Miller¹; Leah V. Schaffer¹; Zach Rolfs¹; Lloyd M. Smith¹;¹ University of Wisconsin, Madison, WI  
| WOB pm 03:10 | Instantly scalable mass spectrometry data storage and inspection in the cloud | Jessica Henning¹,²; Katie Lindner²; Rob Smith²;¹ Prime Labs, Inc., Missoula, MT;² University of Montana, Missoula, MT  
| WOB pm 03:30 | AUTOMATED, WEB-BASED ANALYSIS AND VISUALISATION OF TANDEM ION MOBILITY MASS SPECTROMETRY DATA | Tristan Cragnolin¹,²; Charles Eldrid²; Hannah M. Brit²; Hannes Menneteau²; Aisha Ben-Younis²; Konstantinos Thalassinos¹,²;¹ Birkbeck College, University of London, London, United Kingdom;² University College London, London, United Kingdom  
| WOB pm 03:50 | Graph-based machine learning interprets and predicts diagnostic isomer-selective ion-molecule reactions in tandem mass spectrometry | Jonathan A. Fine¹; Judy K-Y. Liu¹; Armen G. Beck¹; Kawthar Z. Alzarieni¹; Victoria M. Boulou¹; Xin Ma¹; Hilika I. Kenttämaa¹; Gaurav Chopra¹;¹ Purdue University, West Lafayette, IN  
| WOB pm 04:10 | GlyCat: A Skyline tool featuring glycan spectral catalogs for automated analysis and curation of structure data | Christopher Ashwood¹; Rebekah Gundry¹;¹ CardiOomics Program, Center for Heart and Vascular Research; Division of Cardiovascular Medicine; and Department of Cellular and Integrative Physiology, University of Nebraska Medical Center, Omaha, NE, 68198  

*Chair: David Schriemer (University of Calgary)*

*Chair: Riccardo Spezia (Sorbonne Université & CNRS)*
**WOD pm: Imaging: Pharmaceuticals, Metabolites, and Lipids**

Chair: Malcolm Clench (Sheffield Hallam University)

**WOD pm 02:30** Visualizing metabolites related to plant-pathogen interactions with high-resolution AP-SMALDI MSI; Dhaka Bhandari1; Laura Righetti2; Sven Gottwald3; Chiara Dall’asta4; Bernhard Spengler5; 1Justus Leibig University Giessen, Giessen, Germany; 2University of Parma, Parma, Italy

**WOD pm 02:50** Interrogating Skin Cancer Pathology using Mass Spectrometry Imaging; Kelly Dimovska Nilsson1; Noora Neittaanmäki2, 3; Marwa Munem1; Oscar Zaar4, 5; Tina B Angerer6; John Paoli7, 8; John S Fletcher1; 1Department of Chemistry and Molecular Biology, University of Gothenburg, Gothenburg, Sweden; 2Department of Clinical Pathology, Institute of Clinical Sciences, Sahlgrenska Academy, University of Gothenburg, Gothenburg, Sweden; 3Region Västra Götaland, Sahlgrenska University Hospital, Department of Pathology, Gothenburg, Sweden; 4Department of Dermatology and Venereology, Institute of Clinical Sciences, Sahlgrenska Academy, University of Gothenburg, Gothenburg, Sweden; 5Region Västra Götaland, Sahlgrenska University Hospital, Department of Dermatology and Venereology, Gothenburg, Sweden; 6Department of Bioengineering, University of Washington, Seattle, Washington

**WOD pm 03:10** Co-registration of MALDI-MS and LA-ICP-MS images to better understand nanomaterial biodistributions in tissues; Laura Castellanos-Garcia1; Kristen N Sikora1; Richard W Vachet1; 1University of Massachusetts Amherst, Amherst, MA

**WOD pm 03:30** The role of Signaling Sphingolipids in the inflammatory response and granuloma formation during Mtb infection: Potential for new host-directed therapy; Carter Louise Carter1; Veronique Dartois1; 1Hackensack Meridian Health, Nutley, NJ

**WOD pm 03:50** Implementing DESI-MS Imaging in Pharmaceutical Product Development: Methods and Challenges; Josey Ellen Topolski1; Elizabeth Pierson1; 1Merck & Co., Inc., Rahway, NJ

**WOD pm 04:10** On-tissue derivatization techniques for MALDI MS imaging of carbon-carbon double bond positional isomers of phospholipids; Antonin Bednarik1; Jan Preisler1; Dominika Bezděková1; Jiri Stajer1; Vadym Prysiazhnyi1; Michal Hendrych2; Jens Soltwisch3; Klaus Dreisewerd3; 1Department of Chemistry, Masaryk University, Brno, Czech Republic; 2Masaryk University, Brno, Czech Republic; 3Institute of Hygiene, University of Muenster, Muenster, Germany
WOE pm: Hydrogen-Deuterium Exchange MS: Innovations

Chair: Touradj Solouki (Baylor University)

WOE pm 02:30 HDX-MS with electrochemical reduction allows analysis of the insulin-like growth factor receptor and its interaction with blood-brain barrier crossing antibodies; Joey Sheff1; Gerard Comanala2; Feng Ni3; Ping Xu1; Ping Wang1; Melanie Arbour1; Jennifer Hill1; Luke Masson1; Kristin Kemmerich1; John Kelly1; Kasper Rand2; Danica Stanimirovic1; 1National Research Council Canada, Ottawa, ON; 2University of Copenhagen, Copenhagen, Denmark

WOE pm 02:50 Protein Dynamics, Unfolding, and Aggregation: A Thermodynamic Framework for Temperature-Dependent HDX-MS Experiments; Nastaran N. Tajoddin1; Lars Konermann1; 1Univ. of Western Ontario, London, ON

WOE pm 03:10 Hydrogen-Deuterium exchange MS reveals the conformational dynamics of lipopolysaccharide outer membrane insertase LptDE; Francesco Fiorentino1; Joshua B Sauer1; Xing Yu Qiu1; Phillip J Stansfeld2; Jani Reddy Bolla1; Carol V Robinson1; 1University of Oxford, Oxford, United Kingdom; 2University of Warwick, Coventry, United Kingdom

WOE pm 03:30 Remodeling of the Binding Site of Nucleoside Diphosphate Kinase Revealed by X-ray Structure and HDX-MS; Alain Dautant1; Julien Henri2; Philippe Meyer2; Thomas E. Wales3; John R. Engen4; Florian Georgescu5; 1Université de Bordeaux, CNRS, Institut de Biochimie et Génétique Cellulaires, UMR5095, Bordeaux, France; 2Sorbonne Universités, UPMC Univ. Paris 06, CNRS, Laboratoire de Biologie Moléculaire et Cellulaire des Eucaryotes, UMR8226, Institut de Biologie Physico-Chimique, Paris, France; 3Department of Chemistry & Chemical Biology, Northeastern University, Boston, MA

WOE pm 03:50 Integrated structural proteomic techniques shed light on ROty response element recognition and ligand binding; Tim Strutzenberg1; Scott J. Novick1; Ruben Garcia-Ordonez1; Mi Ra Chang1; Patrick R. Griffin1; 1The Scripps Research Institute, Jupiter, FL

WOE pm 04:10 Probing the Fragmentation Mechanisms of Deprotonated Lignin Model Compounds by Using Tandem Mass Spectrometry; Jila Zhang1; Eru Li2; Wanru Li2; John J Nash1; Hilkia I Kettämaa1; 1Purdue University, West Lafayette

WOE pm: Quantitative Proteomics in Systems Biology

Chair: Rena Robinson (Vanderbilt University)

WOF pm 02:30 An Update on the Development of Quantitative MRM Assays for the Large-scale Measurement of Proteins from 20 Mouse Tissues; Sarah A. Michaud1; Angela M. Jackson1; Jamie C. McGuire1; Helena Petrosová1; Yassene Mohammed1, 2; Olga Shevchuk3; Ingo Feldmann3; Albert Sickmann3; Christopher H. Borchers4, 5, 6; 1University of Victoria - Genome British Columbia Proteomics Centre, Victoria, BC; 2Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; 3Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany; 4Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC; 5Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC; 6Department of Data Intensive Science and Engineering, Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow, Russia

WOF pm 02:50 Study design considerations in the quantitative analysis of brain tissue for the analysis of Alzheimer's disease; Gennifer Merrihew1; Julia Robbins1; Jea Park1; Deanna L Plubell1; Vagisha Sharma1; Thomas J. Montine2; Michael J MacCoss2; 1University of Washington, Seattle, WA; 2Stanford University, Stanford, CA

WOF pm 03:10 Beyond BioPlex: Profiling Diversity across Cell-specific Protein Interaction Networks; Laura Pantone Vaites1; David P Nusinow1; Jose Navarrete-Perrea1; Sipei Fu1; Fana Gebreab1; Arvene Golbazi1; Eila Maenpaa1; Keegan Stricker1; Alexandra Thornock1; Sanjukta Guha Thakurta1; Melanie P. Gygi1; Devin K Schwepp1; Joao A. Paulo1; J. Wade Harper1; Steve Gygi1; Edward L. Huttlin1; 1Harvard Medical School, Boston, MA

WOF pm 03:30 Quantitative Top-down MS Analysis of Serum Autoantibody Repertoire in Systemic Lupus Erythematous (SLE); Zhe Wang1; Mulin Fang1; Kellye A Cupp-Sutton1; Xiaowen Liu2; Ken Smith3; Si Wu1; 1University of Oklahoma, Dept. of Chem & Biochem, Norman, OK; 2IUPEI, Indianapolis, IN; 3Oklahoma Medical Research Foundation, Oklahoma City, OK

WOF pm 03:50 Investigating host-pathogen interactions between Apis mellifera and Nosema ceranae using mass spectrometry-based proteomics; Mopelola O. Akinlaja1, 2; Leonard J. Foster1; 1University of British Columbia, Vancouver, BC; 2Michael Smith Laboratories, Vancouver, BC

WOF pm 04:10 The thermal proteome landscape of Escherichia coli; Andre Mateus1; Johannes F. Hevel1; Jacob Bobonis1; Nils Kurzawa1; Malay Shah1; Karin Mitosch1; Camille V. Goemans1; Dominic Helm1; Frank Stein1; Athanasios Typas1; Mikhail M. Savitski1; 1European Molecular Biology Laboratory, Heidelberg, Germany
WOH pm: Environmental: Emerging Contaminants
Chair: Ruth Marfil-Vega (Shimadzu Scientific Instruments)

WOH pm 02:30 LC/QTOF-MS Identifies Unknowns in Wildfire Ash and Water Samples; Michael Thurman1; Imma Ferrer1; Jerry Zweigenbaum2; Sheila F. Murphy3; Jackson P. Webster4; Fernando Rosario-Ortíz5; 1University of Colorado, Boulder, CO; 2Agilent Technologies, Wilmington, DE; 19720; 3U.S. Geological Survey, Boulder, CO; 4California State College, Chico, Chico, CA; 5University of Colorado - Boulder, Boulder, CO

WOH pm 02:50 Confirmation of Contaminants from Serum Suspect Screening Analysis; Ting Jiang1, 2; Miaomiao Wang1; Aolin Wang3; Dimitri Abrahamsson1; Weixin Kuang1, 2; Dana Goin3; Rachel Morello-Frosch3; June-Soo Park1; Tracey Woodruff1; 1California DTSC, Berkeley; 2Public Health Institute, Oakland, CA; 3Department of Obstetrics, Gynecology and Reproductive Sciences, University of California, San Francisco, San Francisco, CA

WOH pm 03:10 Co-occurrence of azole antifungals andazole resistant fungi in wastewater effluents; Hailemariam Abrha Assress1; Hiengilizwe Nyoni1; Bhekizile B Mamba1; Titus Am Msagati1; 1UNIVERSITY OF SOUTH AFRICA(UNISA), JOHANNESBURG, South Africa

WOH pm 03:30 In situ localization of micropollutants and associated stress response in Populus nigra leaves using MALDI-FTICR-imaging and LC-MS/MS.; Claire Villette1; Loïc Maurer1, 2; Julien Delecolle1; Julie Zumsteg1; Mathieu Erhardt1; Dimitri Heinzel1; 1Plant Imaging and Mass Spectrometry (PIMS), Institut de biologie moléculaire des plantes, CNRS, Université de Strasbourg, Strasbourg, France; 2Département technique des fluides et théologie, ICube Laboratoire des sciences de l’ingénieur, de l’infomatique et de l’imagerie, UNISTRA/CNRS/ENGEES/INSA, STRASBOURG, France; 3Institut de biologie moléculaire des plantes (IBMP, CNRS), Strasbourg, France

WOH pm 03:50 Comparison of Computationally Enhanced Non-Targeted Screening Tools: Isotopic Profile Deconvoluted Chromatogram (IPDC) Algorithm and HaloSeeker 1.0; Sadia Fakouri Baygui1; Sébastien Hulin2; Ronan Cariou1; Sujan Fernando1; Philip K. Hopke1; Thomas M. Holsen1; Bernard S. Crimmins1, 3; 1Clarkson University, Potsdam, NY; 2LABERCA Oniris INRAE, Nantes, France; 3AEACS, LLC, New Kensington, PA

WOH pm 04:10 A New Way to Analyze Disinfection By-products in Drinking Water and Complex Matrices with Vacuum Assisted Sorbent Extraction(VASE) and GC-MS; Madison Kilpatrick1; Victoria Noad1; Sage Dunham2; Susan Richardson3; 1University of South Carolina, Columbia, SC; 2Entech Instruments, Simi Valley, CA

WOH pm: Fundamentals for Everyone: Ion Mobility
Chair: Anneli Kruve (Stockholm University)

WOH pm 02:30 Tracking the Structural Evolution of 4-Aminobenzoic Acid in the Transition from Solution to the Gas Phase; Michael Hebert1; David H. Russell2; 1Texas A&M University, DO NOT MAIL, TX; 2Texas A&M University, College Station, TX

WOH pm 02:50 Isolation and characterisation of radical cation species utilising a cyclic ion mobility-enabled quadrupole time-of-flight (Q-cIM-oToF) mass spectrometer; James Scriven1; Jackie Mosely1; Anirudh Sharma1; Martin Palmer2; Jakub Ujma2; Kevin Giles2; Michael J. Bowers2; Kaju Kahn3; Edward Clayton1; 1Teesside University, Middlesbrough, United Kingdom; 2Waters Corporation, Wilmslow, United Kingdom; 3Department of Chemistry and Biochemistry, University of California Santa Barbara, Santa Barbara, CA, 93106-9510; 4Consultant, Macclesfield, United Kingdom

WOH pm 03:10 Elucidating the Gas-phase Unfolding of Protein Complexes through Steered Molecular Dynamics Simulations; Chae Kyung Jeon1; Sugyoun M. Dixit1; Chunyi Zhao1; Brandon T Ruotolo1; 1University of Michigan, Ann Arbor, MI; 2Northwestern University, Chicago, IL

WOH pm 03:30 Deep learning the peptide universe from one million peptide collisional cross sections; Florian Meier1; Niklas D Köhler1; Andreas-David Brunner1; Jean-Marc Wanka2; Eugenia Voytik3; Fabian J Theis2, 3; Matthias Mann1, 4; 1Max Planck Institute of Biochemistry, Planegg, Germany; 2Helmholtz Zentrum München - Institute of Computational Biology, Neuherberg, Germany; 3TU Munich, Munich, Germany; 4Novo Nordisk Foundation Center for Protein Research – University of Copenhagen, Copenhagen, Denmark

WOH pm 03:50 How hot are your ions in differential mobility spectrometry?; Christian leritano1; Joshua Featherstone1; Mircea Guna2; J. Larry Campbell1, 2; W. Scott Hopkins1; 1University of Waterloo, Waterloo, ON; 2SCIEX, Concord, ON

WOH pm 04:10 Pre-processing Ion Mobility Signals: Estimating and Correcting Mobility Shift in Ion Mobility Imaging Mass Spectrometry Experiments; Lukasz Migas1; Emilio Rivera2, 3; Katerina V. Djambazova2, 4; Elizabeth Kathleen Neumann2, 3; Leonoor Ella Marie Timedam1; Nathan Heath Patterson2, 3; Richard M Caprioli2, 3, 4, 5, 6; Jeffrey M Spraggins3, 4, 7; Raf Van De Plass1, 3, 7; 1Delft Center for Systems and Control (DCSC), Delft University of Technology, Delft, Netherlands; 2Mass Spectrometry Research Center, Nashville, TN; 3Department of Biochemistry, Vanderbilt University, Nashville, TN; 4Department of Chemistry, Vanderbilt University, Nashville, TN; 5Department of Medicine, Vanderbilt University, Nashville, TN; 6Department of
Pharmacology, Vanderbilt University, Nashville, TN; Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN
### THURSDAY AM ORALS

#### ThOA am: Instrumentation: Ambient Ionization and Applications

**Chair:** Xin Yan (Texas A&M University)

- **ThOA am 08:30** Multi-functional Vacuum Ionization Source for MAI, LSI, and MALDI: Operational from AP for Comprehensive, Low-Cost Data-Mining in Mass Spectrometry; Sarah Trimpin; Eric T.J. Davis; Abigail Moreno-Pedraza; Calvin A. Austin; Kckenna J. Redding; Monika Kish; Ryan Sohizad; Ahmed Musavi; Frank S. Yenchick; Marcus Simich; Hussein Mokahal; Mary-Kay Pfium; Claudio N. Verani; Trine G. Halvorsen; Scott M. Grayson; Wayne State University, Detroit, MI; MSTM, LLC, Newark, Delaware; Tulane University, New Orleans, LA; University of Oslo, School of Pharmacy, Norway
- **ThOA am 08:50** Methods to enhance collection of out of plane ions in a cycloidal mass spectrometer; Rafael Bento Serna; Elettra Piacentino; Charles B. Parker; Yuriy Zhilichev; Roger P Sperline; Robert Kingston; Scott Tilden; Justin Keogh; Jeffrey T Glass; Jason J Amsden; M. Booner Denton; Duke University, Durham, NC; University of Arizona, Tucson, AZ
- **ThOA am 09:10** Nanodroplets From Submicron Emitters Prevent Clustering during ESI: Evidence for the Serine Octamer in Bulk Solution; Jacob S Jordan; Evan R Williams; University of California, Berkeley, CA; Lawrence Berkeley Laboratory, University of California, Berkeley, California
- **ThOA am 09:30** Multiplexing Electrospray Ionization Sources Using Orthogonal Injection into an Eletrodynamic Ion Funnel; Pei Su; Andrew Jearold Smith; Michael Forrester Espenship; Xi Chen; Hugo Y. Samayoa-Oviedo; Carlos Larriba-Andaluz; Julia Laskin; Purdue University, West Lafayette, IN; Indiana University Purdue University Indianapolis (IUPUI), Indianapolis, IN
- **ThOA am 09:50** Analysis of Non-Conjugated Steroids in Water using Paper Spray Mass Spectrometry; Fred Paul Mark Jjunju; Deidre Erin Damon; Simon Maher; Abraham Badu-Tawiah; University Of Liverpool, Liverpool, United Kingdom; Department of Chemistry and Biochemistry, Ohio State University, Ohio Columbus, Ohio; Department of Electrical Engineering & Electronics, University of Liverpool, Liverpool, United Kingdom; Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH, 43210, USA, Columbus, Ohio
- **ThOA am 10:10** Fiber-based laser ablation electrospray ionization mass spectrometry for molecular profiling and metabolite gradients in anatomical regions selected by fluorescence microscopy; Gessica Vasconcelos; Sylwia Stopka; Gary Stacey; Akos Vertes; George Washington University, Washington, DC; University of Missouri, Columbia, MO

#### ThOB am: Ion Mobility: Small Molecules, Pharmaceuticals, and DMPK

**Chair:** Eleanor Riches (Waters Corporation)

- **ThOB am 08:30** Trapped Ion Mobility Spectrometry (TIMS) and Parallel Accumulation Serial Fragmentation (PASEF) for Urine Metabolomic Profiling; Cristina Di Poto; Matthew Glover; Sonja Hess; Lisa H. Cazares; AstraZeneca R&D, Gaithersburg, MD
- **ThOB am 08:50** Binary Modifiers for Optimized Separation and Sensitivity in Multidimensional Liquid Chromatography/Differential Mobility Spectrometry/Mass Spectrometry; David Ruskie; Gérard Hopfgartner; University of Genève, Geneve, Switzerland
- **ThOB am 09:10** Shining Light on Steroidomics: UV-Catalyzed Reactions to Augment Structural Differences using Ion Mobility-Mass Spectrometry; Samuel W Maddox; Stine S.H. Olsen; Christopher D. Chouinard; Florida Institute of Technology, Melbourne, FL
- **ThOB am 09:30** Characterisation of pharmaceutical formulations enhanced by cyclic ion mobility separation of protomers for tandem mass spectrometry; Jackie A Mosely; James H Scrivens; Anirudh Sharma; Martin Palmer; Jakub Ujma; Kevin Giles; Teesside University, Darlington, United Kingdom; Waters Corporation, Wilmslow, United Kingdom
- **ThOB am 09:50** timsTOF Characterizations of the Esters of Disaccharides and 3-Pyridylboronate in Positive and Negative ESI in situ; Lei Li; Pengfei Guan; Pingping Wang; Jun J Hu; Ningbo University, Ningbo, China
- **ThOB am 10:10** Deviations from the Mason-Schamp Equation for Small Molecules; an Ion Mobility study; Viraj Gandhi; Carlos Larriba Andaluz; IUPUI, Indianapolis, IN; Purdue University, West Lafayette, IN
**ThOD am: Metabolomics: Untargeted Profiling**

Chair: Erica Forsberg (San Diego State University)

**ThOD am 08:30**

**Chemical cartography of the metabolic impact of chronic T. cruzi infection on cardiac tissue:** Danya A Dean\(^1\), 2; Gautham Gautham 3; Jair L Siqueira-Neto 4; James H Mckerrow 4; Pieter C. Dorresteijn 4, 5, 6; Laura-Isobel Mccall 1, 2, 7; 1Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK; 2Department of Biology, University of Oklahoma, Norman, OK; 3Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; 4Center for Microbiome Innovation, University of San Diego, La Jolla, CA; 6Collaborative Mass Spectrometry Innovation Center, University of San Diego, La Jolla, CA; 7Department of Microbiology and Plant Biology, University of Oklahoma, Norman, OK

**ThOD am 08:50**

**Monitoring phenyl-γ-valerolactones production following proanthocyanidins consumption to identify different human gut metabotypes:** Jacob Lessard-Lord 1; Pier-Luc Plante 2; Valentina Cattero 1; Charline Rosine Roussel 1; Stephanie Dudonne 1; Yves Desjardins 1; 1Centre de recherche Nutrition, Santé et Société (NUTRISS), INAF, Université Paris-Saclay, Jouy-en-Josas, France

**ThOD am 09:10**

**Comparison of Three Common Data Acquisition Modes in Liquid Chromatography-Mass Spectrometry Based Untargeted Metabolomics:** Jian Guo 1; Tao Huan 2; 1University of British Columbia, Vancouver, BC

**ThOD am 09:30**

**Combination of UHPLC-MS/MS-molecular networking approach and FTICR-MS for the dereplication of Saccharomyces cerevisiae:** Olivier Perruchon 1; Isabelle Schmitz-Afonso 1; Cécile Grondin 2; Serge Casaregola 3; Carlos Atencia 1; Abdelhakim Elomri 2; 1University of Rouen-Normandy, Mont-Saint-Aignan, France; 2Micalis Institute, INRA, CIRM-Levures, Université Paris-Saclay, Jouy-en-Josas, France

**ThOD am 09:50**

**High Resolution LC-MS Analysis of Wine Samples for the Characterization of Flavanoids:** Brandon Bills 1; Seema Sharma 1; Ralf Tautenhahn 1; Vlad Zabrouskov 1; 1Thermo Fisher Scientific, San Jose, CA

**ThOD am 10:10**

**A library of 400 metabolites for Mapping Metabolome-wide Changes in Cyanobacteria:** Damini Jaiswal 1, 2; Pramod P Wangikar 2; IIT Bombay, Mumbai, India; 2BITS Pilani, Goa, Goa, India; 3Indian Institute of Technology Bombay, Mumbai, India
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<th>Time</th>
<th>Title</th>
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<tr>
<td>ThOF am 08:30</td>
<td>End-to-end automation of multi-attribute method (MAM) platform for process development and characterization of antibodies</td>
<td>Yvonne Ehwang Song¹; Stephen D’eri¹; Martin Hoffmann²; Herve Dubois³; Anja Pfenninger²; Jan Wiesner²; Udo Roth²; Yann Fromentin³; Bradley Whittaker⁴; Marina Hincapie¹; Annette Pieper⁴; Laurent Duhau⁴; Sanofi, Framingham, MA; Sanofi, Frankfurt am Main, Germany; Sanofi, Vitry Sur Seine, France</td>
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<td>ThOE am 08:50</td>
<td>Automated feedback control of protein characteristics in a perfusion bioprocess</td>
<td>James Graham¹; John Schmitt¹; Julia Oddo²; Sylvia Joziak³; Wilfred Tang³; Marshall Berrn³; Eric Carlson³; Brandon Downey³; Lonza, Slough, United Kingdom; Lonza LPB R&amp;D, Bend, Oregon; Protein Metrics Inc., Cupertino, CA</td>
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<td>ThOE am 09:10</td>
<td>High-Throughput, Multi-Attribute Continuous Product Characterisation Platform for Increased Process Control Monitoring</td>
<td>Noemi Dorival-Garcia¹; Patrick Floris¹; Jonathan Bones¹; NIBRT, Dublin, Ireland</td>
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<td>ThOE am 09:30</td>
<td>Point-of-need miniaturized ESI-MS for monitor and control of a bioreactor</td>
<td>Richard W. Moseley¹; Max Wong¹; Alexander I. McIntosh¹; Micrososic Systems, Woking, United Kingdom</td>
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<td>ThOE am 09:50</td>
<td>Quantitative LC-MS/MS workflow for targeted analysis of cell culture media</td>
<td>Hari Kosanam¹; Jared Kress¹; Sha Ha¹; Zuzana Demianova³; Baljit Ubhi³; Lei Xiong³; Merck, WestPoint, PA; Sciex, Brea, CA; SCIEX, Redwood Shores, CA</td>
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<td>ThOE am 10:10</td>
<td>Identification of critical chemical modifications and paratope mapping by size exclusion chromatography (SEC) of stressed antibody-target complexes</td>
<td>Pavel V. Bondarenko²; Gang Xiao¹; Rachel Liuqing Shi¹; Andrew Nichols¹; Thomas M Dillon¹; Pik Becky Chan¹; Margaret S Ricci¹; Amgen, Inc., Thousand Oaks, CA</td>
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<td>ThOF am 08:30</td>
<td>Quantitative Measure of Amiodarone and Associated Metabolites in Single HepG2 Liver Cells Using Single Cell Printing-Liquid Vortex Capture-Mass Spectrometry</td>
<td>John F. Cahill¹; Vilmos Kertesz¹; Oak Ridge National Laboratory, Oak Ridge, TN</td>
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<td>ThOF am 08:50</td>
<td>Single-Cell Mass Spectrometry Reveals Cell-to-Cell Communication in Xenopus laevis (Frog) Embryos</td>
<td>Erika Portero¹; Leena Pade¹; Peter Nemes¹; University of Maryland, College Park, Maryland</td>
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<td>ThOF am 09:10</td>
<td>Single cell mass spectrometry metabolomics studies of cell heterogeneity in the infection of Chagas disease</td>
<td>Yunpeng Lan¹; Tra Nguyen¹; Renmeng Liu¹; Shelley S. Kane¹; Laura-Isobel Mccall¹; Zhibo Yang¹; University of Oklahoma, Norman, OK</td>
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<td>ThOF am 09:30</td>
<td>Combined Single Neuron Patch-Clamp/Mass Spectrometry Analyses</td>
<td>Jolene Diedrich¹; Matt Albertolle³; Nima Dolatabadi¹; Swagata Ghatak¹; Maria Taliantova¹; Stuart A Lipton¹; John Robert Yates III¹; The Scripps Research Institute, La Jolla, CA</td>
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<tr>
<td>ThOF am 09:50</td>
<td>Leveraging trapped ion mobility spectrometry and PASEF for single cell proteomics</td>
<td>Andreas-David Brunner¹; Florian Meier¹; Fabian Coscia¹; Craig Whitehouse¹; Markus Lubeck¹; Nagarjuna Nagaraj¹; Ole Bjeld Hörning³; Oliver Raether³; Andreas Mund³; Nicolai Bache³; Melvin A. Park³; Matthias Mann²; Max Planck Institute of Biochemistry, Planegg, Germany; NNF Center for Protein Research, Copenhagen, Denmark; Bruker Scientific LLC, Billerica, MA; Bruker, Bremen, Germany; Evosep Biosystems, Odense, Denmark</td>
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<td>ThOF am 10:10</td>
<td>Improvements in sensitivity of nanoLC-MS-based deep proteomics profiling using monolithic capillary columns and the FAIMS Pro interface</td>
<td>Michal Gregus¹; Susan E. Abbatiello¹; James Kostas¹; Somak Ray¹; Alexander R. Ivanov¹; Northeastern University, Boston, MA</td>
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**ThOG am: Membrane Protein MS**

Chair: Anumita Saha-Shah (Merck)

- **ThOG am 08:30** "Effect of Nonionic Saccharide Detergents and Supercharging Agents on Native Mass Spectrometry of Membrane Proteins"; Wonhyek Jung; Wenzhe Chen; Muhammad A. Zenaidee; Pascal Egea; Mark Arbing; Rachel R. Ogorzalek Loo; Joseph A. Loo; 1UCLA, Los Angeles, CA

- **ThOG am 08:50** "Uncovering the Molecular Details of G Protein-Coupled Receptor Activation"; Corinne A. Lutomski; Tom N. Durrant; Carol V. Robinson; 1University of Oxford, Oxford, United Kingdom

- **ThOG am 09:10** "Mechanism of adrenergic CaV1.2 stimulation revealed by proximity proteomics"; Marian Kalocsay; Guoxia Liu; Steven O. Marx; Steve Gygi; 1Harvard Medical School, Boston, MA; 2Columbia University College of Physicians and Surgeons, New York, NY

- **ThOG am 09:30** "Top-down high-resolution mass spectrometry of larger membrane proteins: precise subunit mass analysis under conditions that eliminate non-covalent interactions"; Julian Whitelegge; University of California LA, Los Angeles, CA

- **ThOG am 09:50** "Release of membrane proteins from detergent micelles using an in-source declustering ion guide"; Kleitos Sakratous; Jakub Ujma; Kevin Giles; Dale A. Cooper-Shepherd; Ildir Liko; Joseph Gault; Jonathan T. S. Hopper; Carol V. Robinson; 1OMass Therapeutics LTD, Oxford, United Kingdom; 2Waters Corporation, MS Research, Wilmslow, United Kingdom; 3University of Oxford, Oxford, United Kingdom

- **ThOG am 10:10** Empty Slot. Stay tuned for promoted selection to be made.

**ThOH am: Fundamentals: DDA and DIA LC-MS**

Chair: Florian Meier (Jena University Hospital)

- **ThOH am 08:30** "Two-Dimensional Mass Spectrometry, an update"; Anisha Haris; Yuko Lam; Meng Li; Tomos E. Morgan; Bryan P. Marullo; Alina Thiesen; Christopher A. Wootton; Peter B. O’connor; 1University of Warwick, Coventry, United Kingdom; 2Verdel Instruments Ltd, Coventry, United Kingdom; 3University of Warwick, Coventry, United Kingdom

- **ThOH am 08:50** "A Comparison of Intelligent Data-Acquisition Methods for Exposomics and Lipidomics Applications"; Jeremy Koelmel; Georgia Charkoftaki; Sara Nason; Elizabeth Lin; Vasilis Vasiliou; John A. Bowden; Juan Aristizabal; Paul Stelben; Matthew Paige; Krystal G. Pollitt; Timothy J Garrett; 1School of Public Health, Yale University, New Haven, CT; 2Departments of Environmental Sciences and Analytical Chemistry, The Connecticut Agricultural Experiment Station, New Haven, CT; 3Center for Environmental and Human Toxicology & Department of Physiological Sciences, University of Florida, Gainesville, FL; 4Department of Chemistry, University of Florida, Gainesville, FL; 5Department of Pathology, Immunology and Laboratory Medicine, University of Florida, Gainesville, FL

- **ThOH am 09:10** "An ultra-high-resolution IonStar proteomics strategy enables accurate and reproducible large-cohort quantification and outperforms the state-of-the-art SWATH-MS"; Xue Wang; Liang Jin; Chenqi Hu; Shichen Shen; Shuo Qian; Yu Tian; Jun Qu; 1Abbvie, Worcester, Worcester, MA; 2University at Buffalo, Buffalo, NY

- **ThOH am 09:30** "Opportunities and challenges for improving quantitative accuracy and precision in SILAC with DIA-MS"; Lindsay K Pino; Josue Baaza; Richard Lauman; Benjamin A. Garcia; 1Department of Biochemistry and Biophysics, University of Pennsylvania School of Medicine, Philadelphia, PA

- **ThOH am 09:50** "High-field asymmetric waveform ion mobility spectrometry improves the depth and throughput of single-cell proteomics"; Jongmin Woo; Geremy Clair; Chia-Feng Tsai; Sarah M. Williams; Ronald J. Moore; William B. Chrisler; Tao Liu; Richard D. Smith; Ryan T. Kelly; Liljana Pasa-Tolic; Charles K Ansong; Ying Zhu; 1Pacific Northwest National Laboratory, Richland, WA; 2Brigham Young University, Provo, UT

- **ThOH am 10:10** "Lessons Learned the Hard Way: Acquiring and Analyzing Data Independent Acquisition Proteomics Data Collected on Quadrupole-Orbitrap Mass Spectrometers"; Brian C. Searle; Lindsay K Pino; Seth C Just; Michael J MacCoss; 1Institute for Systems Biology, Seattle, WA; 2University of Pennsylvania School of Medicine, Philadelphia, PA; 3Proteome Software, Portland, OR; 4University of Washington School of Medicine, Seattle, Washington
### THURSDAY PM ORALS

**ThOA pm: Pharmaceuticals: Impurity Analysis**  
**Chair:** Miryam Kadkhodaya (Geltor)

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<tr>
<td>02:30</td>
<td>Contribution of FAIMS and DIA for monitoring and accurately quantifying trace-level host cell protein impurities in therapeutic proteins</td>
<td>Nicolas Pythoud¹; Joanna Bons¹; Sega Ndiaye²; Tabiwang Arrey³; Claire Dauly³; Alain Beck⁴; Sarah Cianferrani¹; Christine Carapito¹; University of Strasbourg, CNRS, IRPF, Centre d’Immunologie Pierre-Fabre (CIPF), Saint-Julien-en-Genevois, France</td>
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<td>02:50</td>
<td>Characterization and Quality Control of Synthetic Oligonucleotide Therapeutics by Mass Spectrometry: the Current and the Future</td>
<td>Kui Yang¹; Sarah Rogstad²; Jason Rodriguez¹; David Keire¹; ¹FDA, St. Louis, MO; ²FDA, College Park, MD</td>
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<td>03:01</td>
<td>Accelerated Screening for the Protection and Efficacy of Cell Treatments (ASPECT) via MALDI MS.</td>
<td>Stephen C Zambrycki¹; Gilad Doron²; Monica Tran¹; Carter K Asef¹; Johanna Temenoff²; Facundo M. Fernandez³; School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA; Department of Biomedical Engineering, Georgia Institute of Technology, Atlanta, GA</td>
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<td>03:30</td>
<td>Study of Ranitidine Stability: Quantification of N-Nitrosodimethylamine (NDMA), a Probable Carcinogen in Ranitidine Drug Products and Biological Matrices by UHPLC-MS/MS</td>
<td>Eshani Nandita¹; Ali Najafi²; Neelanagan Bose³; EMERY PHARMA, Alameda, CA; ²Emery Pharma, Alameda, CA</td>
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<td>03:50</td>
<td>A novel data processing strategy for detection of low-abundance HCPs: Increased sensitivity and accuracy with fewer false-positive identifications</td>
<td>Maurizio Bronzetti¹; Jonathan Jones²; Peter Haberl³; Catherine Evans⁴; Stefano Gotta⁴; Genedata Inc, San Francisco, CA; Genedata Ltd, Cambridge, United Kingdom; Genedata GmbH, Munich, Germany; Genedata AG, Basel, Switzerland</td>
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<td>04:10</td>
<td>Rapid Quantitative Analysis of Genotoxic Impurity Nitrosamines in Pharmaceuticals by Liquid Chromatography High Mass Spectrometry</td>
<td>Kate Comstock¹; Christine Skaggs²; Thermo Fisher Scientific, San Jose, CA; Indiana University Purdue University Indianapolis, Indianapolis, IN</td>
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**ThOB pm: Ion Mobility: New Developments & Applications**  
**Chair:** Ian Webb (IUPUI)

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<td>02:30</td>
<td>Surface-induced Dissociation of Trapped Ion Mobility-Selected Protein Complexes</td>
<td>Erin M. Panczyk¹; Dalton T. Snyder¹; Arpad Somogyi¹; Mark E. Ridgeway²; Melvin A. Park²; Vicki H. Wysocki³; The Ohio State University, Columbus, OH; Bruker Daltonics, Billerica, MA</td>
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<td>02:50</td>
<td>Millisecond Chiral Separation by Multidimensional IM-MS Provides Molecular and Structural Basis for Next-generation Therapy of Alzheimer’s Disease</td>
<td>Gongyu Li¹; Min Ma¹; Chae Kyung Jeon²; Brandon T Ruotolo²; Lingjun Li¹; University of Wisconsin-Madison, Madison, Wisconsin; University of Michigan, Ann Arbor, MI</td>
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<td>03:10</td>
<td>Fourier Transform Ion Mobility Linear Ion Trap Mass Spectrometer with Frequency Encoding to Recognize Related Compounds in a Single Acquisition</td>
<td>Robert Schrader¹; Brett M. Marsh¹; R. Graham Cooks¹; Purdue University, West Lafayette, IN</td>
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<td>03:30</td>
<td>Some illustrations of the advances brought by high-resolution ion mobility coupled to multi-function MS capabilities in structural glycoscience</td>
<td>David Ropartz¹,²; Mathieu Fanuel¹,²; Jakub Ujma³; Martin Palmer³; Kevin Giles³; Hélène Rogniaux¹,²; INRAE, UR BIA, Nantes, France; INRAE, BIBS facility, Nantes, France; Waters Corporation, MS Research, Wilmslow, United Kingdom</td>
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<td>03:50</td>
<td>Fourier Transform-Ion Mobility-Orbitrap Mass Spectrometry of Carbohydrates: More Signal, More of the Time</td>
<td>Kristin R McKenna¹; Ramanarayanan Krishnamurthy²,³; Charles L. Liotta¹,²; Brian H Clowers¹; Facundo M. Fernandez¹,²; Georgia Institute of Technology, Atlanta, GA; Center for Chemical Evolution, Atlanta, GA; The Scripps Research Institute, La Jolla, CA; Washington State University, Pullman, WA</td>
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<td>04:10</td>
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Stay tuned for promoted selection to be made.
### ThOC pm: Biotherapeutics: Characterization
**Chair: Ganesh Moorthy (Children’s Hospital of Philadelphia)**

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<tr>
<th>Time</th>
<th>Title</th>
<th>Authors</th>
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<tbody>
<tr>
<td>02:30</td>
<td>Assessment and Optimization of Denaturing and Native Microfluidic CE-MS Methods to Characterize Bispecific Antibodies</td>
<td>Laura Herring1; Natalie K Barker1; Joshua Beri2; J. Scott Mellors2; St John Skilton2; Tracy Kuhlman2; Tim Jacobs1;</td>
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<td>1UNC-Chapel Hill, Chapel Hill, NC; 2908 Devices, Inc., Carnboro, NC; 3Protein Metrics Inc, Cupertino, CA; 4Dualogics, LLC, Durham, NC</td>
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<td>02:50</td>
<td>Rapid Characterization of Therapeutic Antibody Charge Variants Using Microchip-Based Imaged cIEF Integrated with High Resolution Mass Spectrometry</td>
<td>Daniel Donnelly1; Bhumit Patel1; Douglas Richardson1; Mariam S Elnaggar2; Christopher Herring2; Scott Mack2; Erik Gentalen2; 1Merck &amp; Co., Inc., Analytical Research and Development, Kenilworth, NJ; 2Intabio, Inc., Newark, CA</td>
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<td>03:10</td>
<td>Human leukocyte antigen II immunopeptidomics in dendritic cells in response to immune-complexes of TNF with anti-TNF biotherapeutics</td>
<td>Andrea Casasola-LaMacchia1; Robert J Seward1; Maria Stella Ritorto1; Gabrielle Bergeron1; Zhaojiang Lu1; Michael Agostino1; Andrew Ciara1; Nathalie Ahyi-Amendah1; Matthew Willetts2; Shourjo Ghose2; Hai-Young Kim1; Tim Hickling1; Hendrik Neubert1; 1Pfizer Inc., Andover, MA; 2Bruker Daltonics, Billerica, MA</td>
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<td>03:30</td>
<td>Development of a SWATH-Mass Spectrometry-based Proteomic Method for the Characterization of CAR-T Cell Therapy</td>
<td>Camille Lombard-Banek1, 2; Edward J Kwee3; Sumona Sarkar4; John T Elliott5; John E Schiel1, 2; 1National Institute of Standards and Technology, Rockville, MD; 2Institute for Bioscience and Biotechnology Research, Rockville, Maryland; 3National Institute of Standards and Technology, Gaithersburg, Maryland</td>
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<td>03:50</td>
<td>Discovery and characterization of a mAb with C-terminal Fc-extension and O-glycosylation</td>
<td>Harsha Gunawardena1; Eric Beil1; Andrew D Mahan1; Elsa Gorre1; Bo Zhai1; Hirsh Nanda1; 1JOHNSON AND JOHNSON, Spring House, PA</td>
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<td>04:10</td>
<td>Analytical characterisation of cell line and sequence differences on final product properties of biotherapeutics</td>
<td>Lewis Elliott Wharram1; Vicky Smith1; Michael Anyadiegwu2; Jodie Clemmit1; John Liddell1; 1CPI, Darlington, United Kingdom</td>
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### ThOD pm: Metabolomics: New Technologies and Applications
**Chair: Sunia Trauger (Harvard University)**

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<td>02:30</td>
<td>Using Complete Hydrogen-Deuterium Exchange to Identify Unknown Compounds in Untargeted HILIC Metabolomics of Mouse Mammary Tumors</td>
<td>Clayton Bioszies1; Brian C Defelice2; Megan R Showalter3; Tong Shen4; Michael R Sa5; Kacey Vandervorst6; Anastasia L Berg6; Kermit L Carraway III6; Tomas Cajka7; Tobias Kind7; Dinesh K. Barupal7; Oliver Fiehn7; 1UC Davis, Davis, CA; 2Chan Zuckerberg Biohub, San Francisco, CA; 3Metabolon, Morrisville, NC; 4West Coast Metabolomics Center, UC Davis, Davis, CA; 5California Northstate University, College of Medicine, Elk Grove, CA; 6Department of Biochemistry and Molecular Medicine, UC Davis, Sacramento, CA; 7Department of Metabolomics and Translational Metabolism, Institute of Physiology CAS, Prague, Czech Republic</td>
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<td>02:50</td>
<td>Combining Credentialing, Ion Mobility Spectrometry, and Tandem Mass Spectrometry (IMS-MS/MS) to Detect, Identify and Validate Metabolites in Untargeted Analyses</td>
<td>James N. Dodds1; Lingjue Wang2; Gary Patti3; Erin S. Baker4; 1North Carolina State University, Raleigh, NC; 2Washington University, St. Louis, St. Louis, MO</td>
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<td>03:10</td>
<td>Application of predicted collisional cross section to metabolome databases to probabilistically describe the current and future ion mobility mass spectrometry</td>
<td>Corey D Broeckling1; Linxing Yao1; Amy Sheffin1; Johannes P.C. Vissers5; Giorgis Issac6; Jeff Goshawk6; Suraj Dhungana6; Robert Plumb7; 1Colorado State University, Fort Collins, CO; 2Waters Corporation, Wilmwood, United Kingdom; 3Waters Corporation, Milford, MA</td>
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<td>03:30</td>
<td>Profiling of small polar metabolites in genetically modified Arabidopsis thaliana samples by capillary ion chromatography HR-MS</td>
<td>Hannah Schöttler1; Heiko Hayen1; 1University of Muenster - Institute of Inorganic and Analytical Chemistry, Münster, Germany</td>
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<td>03:50</td>
<td>MxP® Quant 500 Kit with Waters Xevo® TQ-XS Mass Spectrometry for Standardized and Comprehensive Targeted Metabolomics and Lipidomics</td>
<td>Ulf Sommer1; Hai Pham-Tuan2; Xenia Enkelmann1; Doreen Kirchberg1; Martin Buratti1; Andrew J. Peck2; Therese Koal1; 1BIOCRATES Life Sciences AG, Innsbruck, Austria; 2Waters Corporation, Milford, Massachusetts</td>
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<td>04:10</td>
<td>Empty Slot. Stay tuned for promoted selection to be made.</td>
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ThOE pm: Protein-Ligand Interactions

Chair: Tracie Williams (Centers for Disease Control and Prevention)

ThOE pm 02:30 Unraveling the Three-dimensional Molecular Recognition Codes of Experimental and Diagnostic Antibodies by nanoESI Ion Mobility Mass Spectrometry; Bright D. Danquah1; Claudia Röwer1; Kwabena F.M. Opuni1; Reham A. El-Kased2; Cornelia Kov1; Michael O. Glocker1; 1Proteome Center Rostock, Rostock, Germany; 2School of Pharmacy, University of Ghana, Legon, Ghana; 3The British University in Egypt, Cairo, Egypt

ThOE pm 02:50 Native Top-Down Mass Spectrometry of Amyloid Proteins and Their Interaction with the Aggregation Inhibiting Compound CLR01; Carter Lantz1; Muhammad A. Zenaidee1; Jaybree Lopez1; Rachel R. Ogorzalek Loo1; Gal Bitan1; Joseph A. Loo1; 1University of California, Los Angeles, Los Angeles, CA

ThOE pm 03:00 Assembly and regulation of the chlorhexidine specific efflux pump AceI; Jani Reddy Bolla1; Anna C Howes1; Francesco Fiorentino1; Carol V Robinson1; 1University of Oxford, Oxford, United Kingdom

ThOE pm 03:30 Peanut allergen ejection for unambiguous characterization of immunological interactions; John P Mcgee1; Rafael D Melani1; Valerie J Winton1; Derek Croote2; Benjamin Des Soye1; Michael A Swift2; Stephen R Quake2; Neil L. Kelleher1; Philip D Compton1; 1Northwestern University, Evanston, IL/60208; 2Stanford University, Palo Alto, CA

ThOE pm 03:50 Probing Host-Microbe Interactions Through Glycomic and Glycoproteomic Methods; Ying Sheng1; Yixuan (axe) Xie1; Qiongyu Li1; Carlito B Lebrilla1; 1University of California, Davis, Davis, CA

ThOE pm 04:10 Determining the Binding Site of Molecules on A424 by DFT Calculations and Fast Photochemical Oxidation of Proteins (FPPOP) Mass Spectrometry; George Mathai1; Saketh Chemuru2; Daryl Giblin2; Michael L. Gross2; 1Sacred Heart College, Kochi, India; 2Department of Chemistry, Washington University in St. Louis., st. Louis, Missouri

ThOF pm: Carbohydrates

Chair: Yehia Mechref (Texas Tech University)

ThOF pm 02:30 EED MS2-guided -MS3 on Q Exactive-Omnitrap: a novel approach toward automated, de novo glycan sequencing; Juan Wei1; Dimitris Papanastasiou2; Mariangela Kosmopoulou2; Athanasios Smyrnakis2; Yang Tang1, 3; Joseph Zaia1; Pengyu Hong1; Catherine E. Costello1, 3; Cheng Lin1; 1Center for Biomedical Mass Spectrometry, Boston University School of Medicine, Boston, MA; 2Fasmatech Science and Technology, Athens, Greece; 3Department of Chemistry, Boston University, Boston, MA; 4Department of Computer Science, Brandeis University, Waltham, MA

ThOF pm 02:50 Glycoproteomic and imaging MS applications of an alpha 2,3 linked sialic acid targeted bioorthogonal chemical labeling probe; Richard R Drake1; Colin Modoweli1; Connor A West1; Grace Grimsley1; Xiaowei Lu1; 1Medical University of South Carolina, Charleston, SC

ThOF pm 03:10 MOBILion’s SLIM-Mass Spectrometry for High Resolution and High Throughput Ion Mobility Analyses of N- and O-linked Glycoprotein Glycans; Lance Wells1; Kelly L. Wormwood Moser2; James R. Arndt2; Anisha Yadav2; Stephen Kruka2; Gregory Van Aken2; John Daniel DeBord2; Gregory Webster2; Robert Bridger1; Kazuhiro Aoki1; Jeremy Praissman1; Laura Maxon1; Michael Tiemeyer1; 1CCRC/UGA, Athens, GA; 2MOBILion Systems Inc., Chadds Ford, PA

ThOF pm 03:30 Advances in Tandem Mass Spectrometry Approaches for the Structural Characterization of Sulfated Glycosaminoglycans; Lauren E. Peri1; Zachary J. Sasiene2; Franklin E. Leach III1; Praneeth M. Mendis2; Dustin R. Klein3; Pradeep Chopra4; Fuming Zhang3; Robert J. Linhardt4; Geert-Jan Boons4; Jennifer S. Brodbelt4; Glen P. Jackson3; I. Jonathan Amster1; 1University of Georgia, Athens, GA; 2West Virginia University, Morgantown, WV; 3Vanderbilt University, Nashville, TN; 4Complex Carbohydrate Research Center, University of Georgia, Athens, GA; 5Rensselaer Polytechnic Institute, Troy, NY; 6University of Texas at Austin, Austin, TX

ThOF pm 03:50 Differentiating Fragmentation Pathways of Sialylated Human Milk Oligosaccharides as Magnesium Adducts by Electron Transfer/Ion Mobility/Vibrational Activation; Anna J Diepenbrock1; Eric D Dodds2; 1University of Nebraska - Lincoln, Lincoln, NE; 2University of Nebraska-Lincoln, Lincoln, NE

ThOF pm 04:10 Resolving positional and compositional isomers of protonated disaccharides by tandem mass spectrometry, ion mobility, and gas-phase hydrogen deuterium exchange; Abhiyaa Mookherjee1; Sanjit (sunny) Uppal2; Miklos Gutman2; 1University of Washington, Seattle; 2University of Washington, Seattle, Seattle, WA
ThOG pm: Synthetic Polymers

Chair: Kevin Endres (E. I. du Pont de Nemours and Company)

ThOG pm 02:30 Differences in MALDI ionization of neat linear and cyclic poly(L-lactide); Steffen M Weidner¹; Hans R. Kricheldorf²; ¹Federal Institute for Materials Research & Testing, Berlin, Germany; ²Universität Hamburg, Hamburg, Germany

ThOG pm 02:50 Comprehensive characterization of poly(lactide-co-glycolide)s combining chromatography with matrix- and surface-assisted laser desorption ionization low- and high-resolution mass spectrometry; Thierry Nicolas Jean Fouquet¹; Takayuki Ohmura²; Masataka Kotani²; Yasuhide Naito³; Delphine Crozet⁴; Pierre Giusti⁵,⁶; Laurence Charles⁷; ¹National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan; ²Hamamatsu Photonics K.K., Iwata, Japan; ³The Graduate School for the Creation of New Photonics Industries, Hamamatsu, Japan; ⁴Total Refining and Chemicals, Harfler, France; ⁵International Joint Laboratory - IC2MC: Complex Matrices Molecular Characterization, Harfler, France; ⁶Aix-Marseille Université - Institut de Chimie Radiculaire, Marseille, France

ThOG pm 03:10 Rethinking the Structure and Reactivity of Silicone MQ Resins; Richard Cooper¹; Tianlan Zhang²; Steven Arturo¹; ¹Dow, Collegeville, PA; ²Glaukos Corporation, San Clemente, California

ThOG pm 03:30 Regio and stereospecific chemical depolymerization of high molecular mass polybutadiene and polyisoprene for the analysis by high resolution mass spectrometry; Ziad Mahmoud¹; Fabrice Bray¹; Marie Hubert-Roux²; Michel Sablier³; Carlos Alfonso⁴; Christian Rolando⁵; ¹Université de Lille, Faculté des Sciences et Technologies, USR 3290 MSAP, Miniaturisation pour l’Analyse, la Synthèse et la Protéomique, 59655 Villeneuve d’Ascq Cedex, France; ²Villeneuve d’Ascq Cedex, France; ³University of Rouen, UMR 6014, CNRS, COBRA, Chimie organique et bioorganique, Réactivité et Analyse, 76821 Mont-Saint-Aignan Cedex, France, Rouen, France; ⁴Muséum National d’Histoire Naturelle, USR 3224, CNRS, Centre de Recherche sur la Conservation, 36, rue Geoffroy Saint-Hilaire, 75005 Paris, France

ThOG pm 03:50 Empty Slot. Stay tuned for promoted selection to be made.

ThOG pm 04:10 Empty Slot. Stay tuned for promoted selection to be made.

ThOH pm: Fundamentals for Everyone: Imaging

Chair: Nathalie Agar (Harvard University)

ThOH pm 02:30 Exploratory and Predictive Analysis of Imaging MS Data: Machine Learning Approaches; Raf Van de Plas¹,²,³; Lukasz G. Migas¹; Leonoor E.M. Tideman¹; Emilio S. Rivera²,³; Katerina V. Djambazova²,⁴; Elizabeth K. Neumann²,³; N. Heath Patterson²,³; Jeffrey M. Spraggins²,³,⁴; Richard M. Caprioli²,³,⁴,⁵,⁶; ¹Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; ²Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ³Department of Biochemistry, Vanderbilt University, Nashville, TN; ⁴Department of Chemistry, Vanderbilt University, Nashville, TN; ⁵Department of Pharmacology, Vanderbilt University, Nashville, TN; ⁶Department of Medicine, Vanderbilt University, Nashville, TN

ThOH pm 02:50 Performance Evaluation of a MALDI LTQ Orbitrap XL Imaging Platform Interfaced with a Next-Generation Data Acquisition System; Konstantin O. Nagornov¹; Anton N. Kozhinov¹; Franklin E. Leach III²; Yury O. Tsybin¹; ¹Spectroswiss, Lausanne, Switzerland; ²University of Georgia, Athens, GA

ThOH pm 03:10 Measuring spatial resolution in Mass Spectrometry Imaging – development of parametric and non-parametric approaches; Martin Melotiey¹,²; Rory T Steven¹; Xavier Loizeau¹; Alex Dexter¹; Chelsea Nikula¹; Ammar Nasif¹; Kenneth Robinson¹; Bin Yan¹; Zoltan Takats²; Josephine Bunch¹,²; ¹NPL, Teddington, United Kingdom; ²Imperial College London, London, United Kingdom

ThOH pm 03:30 Tandem mass tag labeling enables high throughput imaging of 2000 proteins at 50-µm spatial resolution from tissue sections; Ying Zhu¹; Paul D Piekowski¹; Yang Wang¹; Kelly G Stratton¹; Sarah M. Williams¹; Jia Yuan²; Sudhansu K Dey²; Ronald J. Moore¹; Richard D. Smith¹; Lisa M Bramer¹; Kristin E Burnum-Johnson¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²Cincinnati Children’s Hospital Medical Center, Cincinnati, OH

ThOH pm 03:50 Discovering powerful biocatalysts with a novel platform combing microdroplet-printing and microscale mass spectrometry imaging; Linfeng Xu¹; Lejian Liu¹; Adam Abate¹,²; Nannan Tao³; Shannon Cornett¹; ¹University of California San Francisco, San Francisco, CA; ²Chan Zuckerberg Biohub, San Francisco, CA; ³Bruker Scientific, San Jose, CA; ⁴Bruker Scientific LLC, Billerica, MA

ThOH pm 04:10 Development of an Instrument Optimized for Multiplexed Ion Beam Imaging of 2D Tissue Samples; Elizabeth R Schemm¹; Ben Shepperson¹; Jay G Tarolli¹; Steve P Thompson¹; Rich Tighe¹; ¹IONpath, Menlo Park, CA