



JUNE 2-6

2024

ANAHEIM
CALIFORNIA

ORALS

This document includes a detailed schedule for the parallel oral sessions, Monday – Thursday.

A final program (PDF) will be created over the coming weeks and will combine this document with a schedule overview, posters, workshops, and an author index.

Conference attendees are encouraged to use the digital conference program tools, Planner & App, available here:

<https://www.asms.org/conferences/annual-conference/online-planner-app>

MONDAY ORALS

MOA am: Metabolomics: Untargeted Profiling Room 210ABC (Level 2)

Session Chair: Jessica Prenni (Colorado State University)

- MOA am 08:30 **3D Molecular Cartography of the International Space Station**; Haogqi Nina Zhao¹; Rodolfo A. Salido²; Helena Mannocho-Russo¹; Simone Zuffa¹; Rob Knight^{2, 3, 4, 5}; Pieter C. Dorrestein^{1, 4, 6, 7}; ¹Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; ²Department of Bioengineering, University of California San Diego, La Jolla, CA; ³Department of Pediatrics, University of California San Diego, La Jolla, CA; ⁴Center for Microbiome Innovation, University of California San Diego, La Jolla, CA; ⁵Department of Computer Science and Engineering, University of California San Diego, La Jolla, CA; ⁶Department of Pharmacology, University of California San Diego, La Jolla, CA; ⁷Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA
- MOA am 08:50 **Dietary Iron Intake Modulates Fecal Metabolome and Microbiome**; Anastasia Kostenko¹; Simone Zuffa^{2, 3}; Hui Zhi⁴; Kevin Mildau^{5, 6}; Manuela Raffatellu^{2, 4}; Pieter Dorrestein^{2, 3}; Allegra Aron^{1, 2, 3}; ¹University of Denver, Denver; ²Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; ³Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; ⁴Department of Pediatrics, University of California San Diego, La Jolla, CA; ⁵Department of Analytical Chemistry, University of Vienna, Vienna, Austria; ⁶Bioinformatics Group, Wageningen University & Research, Wageningen, Netherlands
- MOA am 09:10 **Metabolomics of 13,700 human plasma samples for the TEDDY cohort: A Big Data Challenge and Opportunity for Mass Spectrometry**; Uri Keshet¹; Bashar Amer²; Gert Wohlgemuth¹; Yuanyue Li¹; Iris Beussen¹; Jeremiah Wells¹; Carol Stroble¹; Oliver Fiehn¹; ¹University of California Davis, Davis, CA; ²ThermoFisher Scientific, San Jose, CA
- MOA am 09:30 **Longitudinal Monitoring of Human Urine Metabolites**; Corinne E Moss¹; Katherine A Overmyer^{1, 2}; J. Will Thompson³; Hampus Engstrom³; Ian J Miller¹; Emily Lohr¹; Nicole M Nightingale²; Scott J Mellors³; Joshua J Coon^{1, 2}; ¹University of Wisconsin-Madison, Madison, WI; ²Morgridge Institute for Research, Madison, WI; ³908 Devices, Boston, MA
- MOA am 09:50 **A Mechanistic Understanding of Post-Acquisition Sample Normalization for Untargeted Metabolomics**; Brian Low¹; Huaxu Yu¹; Tao Huan¹; ¹University of British Columbia, Vancouver, BC
- MOA am 10:10 **Development of Mass Spectral Libraries with Precursor and Fragment Annotated Mass Spectra to Improve Identifications of Metabolites**; Xinjian Yan; National Institute of Standards and Technology, Gaithersburg, MD

MOB am: Glycopeptides, Glycoproteins, and Glycomics Room 207ABC (Level 2)

Session Chair: Parastoo Azadi (University of Georgia)

- MOB am 08:30 **ExD fragmentation facilitates high-confidence characterization of intact N- and O-linked glycopeptides**; Chaoshuang Xia¹; Margaret Downs¹; Juan Wei²; Joseph Zaia¹; Cheng Lin¹; Catherine E. Costello¹; ¹Center for Biomedical Mass Spectrometry, Boston University Chobanian and Avedisian School of Medicine, Boston, Massachusetts; ²School of Pharmaceutical Sciences, Shanghai Jiao Tong University, Shanghai, China

- MOB am 08:50 **Exploring the Mucinome of Synovial Fluid and Plasma in Osteoarthritis**; Vincent Chang¹; Ellie Browne¹; Keira E. Mahoney¹; Taryn M. Lucas¹; Niclas G. Karlsson²; Stacy A. Malaker¹; ¹Yale University, New Haven, CT; ²Oslo Metropolitan University, Oslo, Norway
- MOB am 09:10 **Extracting informative glycan-specific ions from glycopeptide MS/MS spectra using GlyCounter**; Anna G. Duboff¹; Kathryn Kothlow¹; Kayla A. Markuson¹; Jacob H. Russell¹; Emmajay Sutherland¹; Tim S. Veth¹; Ruby Zhang¹; Nicholas M. Riley¹; ¹University of Washington, Seattle, WA
- MOB am 09:30 **Profiling N-glycans and identifying their attachment site on glycoRNAs using DIA-MS**; Yixuan (Axe) Xie¹; Helena Hemberger^{2, 3}; Xingyu Liu¹; Nicholas Till⁴; Peiyuan Chai^{2, 3}; Christopher Watkins^{2, 3}; Charlotta Lebedenko^{2, 3}; Zongtao Lin¹; Reese Caldwell^{2, 3}; Benson George^{2, 3}; Carolyn R. Bertozzi⁴; Ryan A. Flynn^{2, 3}; Benjamin A. Garcia¹; ¹Washington University School of Medicine, St. Louis, MO; ²Boston Children's Hospital, Boston, USA, MA; ³Harvard University, Cambridge, MA; ⁴Stanford University, Stanford, CA
- MOB am 09:50 **High-Quality Human Plasma N-Glycoproteomics on a ZenoTOF using optimized combinations of CID and electron activated dissociation (EAD)**; Shelley Jager¹; Tatiana M. Shamorkina¹; Sibylle M. Heidelberger²; Heather Chassaing²; Karli R. Reiding¹; Albert J.R. Heck¹; ¹Utrecht University, Utrecht, Netherlands; ²SCIEX, Macclesfield, United Kingdom
- MOB am 10:10 **Mass spectrometric analysis of glycopeptides enriched by anion exchange-mediated methods reveals polyLacNAc-extended N-glycans in melanoma cells**; Maryam Baniasad¹; Gege Xu¹; Tomislav Čaval¹; Chih-Wei Chu¹; Rachel Rice¹; Itati Hundal¹; Gregg Czerwieńiec¹; Xin Cong¹; Flavio Schwarz¹; ¹InterVenn Biosciences, South San Francisco, CA

MOC am: Fundamentals Beyond Mass Analysis: Isomers Room 304AB (Level 3)

Session Chair: Yu Xia (Tsinghua University)

- MOC am 08:30 **Decoding Prototropic Isomers of Fentanyl Analogs using Ion Mobility, Tandem Mass Spectrometry, and Computational Approaches**; Ralph Aderorho¹; Christian Ieritano²; Copeland R. Johnson¹; W. Scott Hopkins²; Christopher D. Chouinard¹; ¹Clemson University, Clemson, SC; ²University of Waterloo, Waterloo, ON
- MOC am 08:50 **Measurable Influences of the Electrospray Solvent on Small Molecule Collision Cross Sections in Ion Mobility: the Possible Role of Protomers**; Nadjali A Chung¹; Jody C May^{1, 2}; Renā AS Robinson¹; John A McLean^{1, 2}; ¹Department of Chemistry, Vanderbilt University, Nashville, TN; ²Center for Innovative Technology, Nashville, TN
- MOC am 09:10 **Experiment and Theory of High-Resolution Ion Mobility and Cryogenic Infrared Spectroscopic Measurements to Resolve and Identify Isomeric Compounds**; Christopher Harrilal¹; Sean M. Colby²; Jessica L. Bade²; Peter S. Rice²; Amy M. Jystad²; Sandilya V. Garimella²; Simone Raugeri²; Yehia M. Ibrahim²; ¹Pacific Northwest National Lab, Richland, WA; ²PNPL, Richland, WA
- MOC am 09:30 **Rapid Quantification and Molecular Imaging of Fatty Acid Isomers with Dual-Resolved C=C Bond Geometry and Position by Ion Mobility-Mass Spectrometry**; Zhijun Zhu¹; Shuling Xu¹; William J. Heelan¹; Hua Zhang¹; Penghsuan Huang¹; Gaoyuan Lu¹; Amy B. Banta¹; Jason M. Peters¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI

MONDAY ORALS

- MOC am 09:50 **Multi-level protein structure governs aspartic acid isomerization in vitro**; Thomas A Shoff¹; Vivian C Onwudiwe¹; Joseph Genereux¹; Ryan R. Julian¹; ¹University of California, Riverside, Riverside, CA
- MOC am 10:10 **Exploration of unusual covalent bond cleavages upon dissociation of diastereomeric magnesium complexes for chiral isomer discrimination**; Chenqin CAO¹; Sandra ALVES²; Yves GIMBERT^{2,3}; Jean-Claude Tabet^{1,2}; Christophe JUNOT¹; François FENAILLE¹; Annelaure DAMONT¹; ¹Université Paris-Saclay, CEA, INRAE, Département Médicaments et Technologies pour la Santé (DMTS), MetaboHUB, Gif-sur-yvette, France; ²Sorbonne Université, Faculté des sciences et de l'ingénierie, Institut Parisien de Chimie Moléculaire (IPCM), Paris, France; ³Département de Chimie Moléculaire, UMR CNRS 5250, Université Grenoble Alpes, Grenoble, France
- MOD am 10:10 **Tracking the Metabolome and Proteome changes of a soil microbiome during the evolutionary adaptation against agrochemicals**; Karoline Steuer-Lodd¹; Paolo Stincone^{2,3}; Lukas Miles Braun²; Abzer Kelimal Pakkir Mohamed Shah³; Marcelo Navarro Diaz³; Silvana Teresa Tapia Paniagua⁴; Eric Kemen²; Daniel Petras¹; ¹University of California, Riverside, Riverside, CA; ²University of Tuebingen, Center for Plant Molecular Biology, Tübingen, Germany; ³University of Tuebingen, CMFI Cluster of Excellence, Interfaculty Institute of Microbiology and Infection Medicine, Tübingen, Germany; ⁴University of Malaga, Faculty of Science, Department of Microbiology, Malaga, Spain
- MOD am: Microbes and the Microbiome**
Room 304CD (Level 3)
 Session Chair: Emma Guiberson (Stanford University)
- MOE am: Instrumentation: Ambient Ionization and Applications**
Ballroom DE (Level 3)
 Session Chair: Cheng-Chih Richard Hsu (National Taiwan University)
- MOD am 08:30 **Insights into Gut Microbiome Metabolism Revealed through Untargeted Metabolomics and Molecular Networking**; Mark Sartain¹; James S Pyke¹; Emma E. Rennie¹; Elizabeth Almasi¹; Ruben J.F. Ramos²; Sara Nunes Violante²; Justin R Cross²; ¹Agilent Technologies, Santa Clara, CA; ²Donald B. and Catherine C. Marron Cancer Metabolism Center, Memorial Sloan Kettering Cancer Center, New York, NY
- MOD am 08:50 **Comparative analysis of vaping in PWH reveals systemic metabolome alterations and links novel microbial derived metabolite, DHPS, to metabolic dysregulation**; Courtney J Christopher¹; Aline Zaparte²; Lauren Richey³; Connie Arnold³; Chris Taylor⁴; Adairre Castille²; Hui-yi Lin⁵; John P Kirwan⁶; John W Apolzan⁶; David A Welsh²; Shawn R. Campagna^{1,7}; ¹University of Tennessee Knoxville Chemistry Dept., Knoxville, TN; ²Louisiana State University Department of Medicine, New Orleans, LA; ³Louisiana State University, New Orleans, LA; ⁴Louisiana State University Department of Microbiology, Parasitology & Immunology, New Orleans, LA; ⁵Louisiana State University School of Public Health, New Orleans, LA; ⁶Pennington Biomedical Research Center, Baton Rouge, LA; ⁷Biological Small Molecule Mass Spectrometry Core, Knoxville, Tennessee
- MOD am 09:10 **Quantitative multilevel proteomics to characterize an intestinal epithelial model for application in assessing host-microbiome-drug interactions**; Emily Fekete¹; Marybeth Creskey¹; Angela Wang¹; Xu Zhang¹; ¹Health Canada, Ottawa, ON
- MOD am 09:30 **Effect of Synbiotic Treatment on Fecal Metabolome in Infants with Cow's Milk Allergy**; Mariyana V Savova¹; Pingping Zhu¹; Alida Kindt¹; Harm Wopereis²; Clara Belzer³; Amy C. Harms¹; Thomas Hankemeier¹; ¹Metabolomics and Analytics Centre, Leiden Academic Centre of Drug Research, Leiden University, Leiden, Netherlands; ²Danone Nutricia Research, Utrecht, Netherlands; ³Laboratory of Microbiology, Wageningen University, Wageningen, Netherlands
- MOD am 09:50 **Culture-Independent Identification of Microbes in Seconds Directly from Clinical Samples using the MasSpec Pen Technology**; Manoj Kumar¹; Coreen L. Johnson²; Michael Keating³; James J. Dunn²; Faith Jackobs³; Rachel D. Downey⁴; Lindsey M. Kirkpatrick⁵; Livia S. Eberlin⁶; ¹Baylor College of Medicine, Dept. of Surgery, Houston, Texas; ²Texas Children's Hospital, Dept. of Pathology, Houston, Texas; ³Baylor College of Medicine, Houston, Texas; ⁴Dell Children's Medical Center, Austin, Texas; ⁵Riley Hospital for Children, Dept. of Pediatric Infectious Diseases, Indianapolis, Indiana; ⁶Baylor College of Medicine, Dept. of Surgery, Houston, Texas
- MOE am 08:30 **Use of Matrix Assisted Ionization in Vacuum-Mass Spectrometry to Characterize the Surface Layers of Organic Particles**; Lisa M Wingen¹; Yiming Qin²; Véronique Perraud¹; Styliani Consta³; Barbara J Finlayson-Pitts¹; ¹University of California, Irvine, Irvine, CA; ²City University of Hong Kong, Hong Kong, Hong Kong; ³University of Western Ontario, London, Ontario
- MOE am 08:50 **Triboelectric Nanogenerator Plasma Ionization for Portable VOC Analysis**; Joseph Corstvet¹; Wesley D. Roberston¹; Facundo M. Fernandez¹; ¹Georgia Institute of Technology, Atlanta, GA
- MOE am 09:10 **Understanding The Cellular Metabolism: High-Throughput Profiling of Intact Cells using Laser Desorption-Rapid Evaporative Ionization Mass Spectrometry (LD-REIMS)**; Stefania Maneta-Stavarakaki¹; Annalisa Lorenzato²; Adrienn Molnar³; Daniel Simon¹; Yuchen Xiang¹; Mariangela Russo²; Clelia Nisticò^{2,4}; Laura Bizzozero⁴; Andrew Campbell⁵; Julia Balog⁶; Owen Sansom⁵; Sabrina Arena^{2,4}; Alberto Bardelli²; Zoltan Takats¹; ¹Department of Metabolism Digestion and Reproduction, Imperial College London, London, United Kingdom; ²Department of Oncology, University of Torino, Candiolo, Italy; ³Hevesy György PhD School of Chemistry, ELTE Eötvös Loránd University, Budapest, Hungary; ⁴Candiolo Cancer Institute, FPO - IRCCS, Laboratory of ,Translational Cancer Genetics, Candiolo, Italy; ⁵The Beatson Institute, Glasgow, United Kingdom; ⁶Waters Corporation, Milford, Massachusetts
- MOE am 09:30 **Rapid onsite analysis with Temperature-tuning desorption ionization and miniature mass spectrometer**; Qiong Liang¹; Xinwei Liu²; Junlong Hong¹; Jiexun Bu¹; Zheng Ouyang²; ¹PURSPEC Technology (Beijing) Ltd., Beijing, China; ²Tsinghua University, Beijing, China
- MOE am 09:50 **Spatially-resolved top-down proteomics of human skin using probeform imaging mass spectrometry (PIMS)**; Vijaya Lakshmi Kanchustambham¹; Pei Su¹; Tian Xu¹; Michael A. R. Hollas¹; Korvell Russell²; Bethany Perez White²; Michael A. Caldwell¹; Jared Otto Kafader¹; Neil L. Kelleher¹; ¹Northwestern University, Evanston, IL; ²Northwestern University, Feinberg School of Medicine, Chicago, IL
- MOE am 10:10 **A Need for Speed: Laser Heating to Investigate the Thermal Stability and Aggregation Kinetics of Fast Forming Protein Oligomers**; Jacob S Jordan¹; Katherine J Lee¹; Evan R Williams¹; ¹University of California, Berkeley, Berkeley, CA

MONDAY ORALS

MOF am: Nucleic Acids and Oligonucleotides Ballroom C (Level 3)

Session Chair: Varun Gadkari (University of Minnesota)

- MOF am 08:30 **Improved Characterization of Heavily-Modified RNA Therapeutics through Activated-Ion Negative Electron Transfer Dissociation (AI-NETD);** Daniel Jacob Nesbitt¹; Trenton M. Peters-Clarke¹; Keaton L. Mertz¹; Scott T. Quarmby^{2,3}; Trent J. Oman⁴; Joshua J. Coon^{1,2,3,5}; ¹Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ²National Center for Quantitative Biology of Complex Systems, Madison, WI; ³Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; ⁴Eli Lilly & Company, Indianapolis, IN; ⁵Morgridge Institute for Research, Madison, WI
- MOF am 08:50 **Mass Spectrometry-Based DNA Methylome Analysis;** Janine F. M. Otto¹; Nico Ueberschaar²; Anne Busch^{3,4}; Michael Bauer^{3,4}; Georg Pohnert^{1,4}; ¹Friedrich Schiller University Jena, Institute of Inorganic and Analytical Chemistry, Jena, Germany; ²Friedrich Schiller University Jena, Mass Spectrometry Platform, Jena, Germany; ³Jena University Hospital, Department of Anaesthesiology and Intensive Care Medicine, Jena, Germany; ⁴Cluster of Excellence Balance of the Microverse, Friedrich Schiller University Jena, Jena, Germany
- MOF am 09:10 **Charge Detection-Mass Spectrometry Enables Molecular Characterization of Nucleic Acid Nanoparticles.;** Polycarp C. Ofoegbu¹; Grant A. Knappe²; Martin F. Jarrold¹; ¹Indiana University Bloomington, Bloomington, IN; ²Massachusetts Institute of Technology, Cambridge, MA
- MOF am 09:30 **Customizable strand-cleaving deoxyribozymes for the mid-down characterization of nucleic acid-based biotherapeutics;** Sarah Mutchek¹; Thomas Kenderdine¹; Daniele Fabris^{1,2}; ¹University of Connecticut, Storrs, CT; ²RiboDynamics, Manchester, CT
- MOF am 09:50 **Ion Mobility Enhanced Top-Down Mass Spectrometry of Large Highly Modified CRISPR gRNA;** Luis A. Macias¹; Ellen Rohde¹; James A. Madsen¹; ¹Verve Therapeutics, Boston, MA
- MOF am 10:10 **Analytical characterization of divalent siRNA via liquid chromatography and mass spectrometry;** Molly S. Blevins¹; Jenny Wang¹; Stefan G. Koenig¹; Kelly Zhang¹; ¹Genentech, South San Francisco, CA

MOG am: Data-Independent Acquisition and Multiplexing Ballroom AB (Level 3)

Session Chair: Claire Eyers (University of Liverpool)

- MOG am 08:30 **Synchronizing the TIMS ramp with the quadrupole scan demonstrates a significant qualitative and quantitative improvement in DIA analysis;** Oliver M. Bernhardt¹; Sander Willems²; Christopher Below³; Roland Bruderer¹; Dennis Trede⁴; Tejas Gandhi¹; Lukas Reiter¹; ¹Biognosys AG, Schlieren, Switzerland; ²Bruker, Kontich, Belgium; ³Biognosys, Schlieren, Switzerland; ⁴Bruker Daltonics GmbH & Co. KG, Bremen, Germany
- MOG am 08:50 **mTIFF: multiplexed transferring identification based on FAIMS filtering enhances throughput and sensitivity of single-cell proteomics;** Yumi Kwon¹; Fengchao Yu²; Sarah M. Williams¹; Ljiljana Paša-Tolić¹; Alexey I. Nesvizhskii^{2,3}; Ying Zhu⁴; ¹Pacific Northwest National Laboratory, Richland, WA; ²Department of Pathology, University of Michigan, Ann Arbor, Michigan, 48109-1382, United States, Ann Arbor, MI; ³Department of Computational Medicine and Bioinformatics, University of Michigan, Ann Arbor, Michigan, 48109-1382, United States, Ann Arbor, MI; ⁴Genentech Inc, South San Francisco, CA

- MOG am 09:10 **The Screen's Gambit: Functional Chemoproteomics Accelerated by Compressed Sensing and Generative Models;** Carolyn Allen¹; J. Sebastian Paez¹; Andrea I. Gutierrez¹; Julia E. Robbins¹; Daniele Canzani¹; Lindsay K. Pino¹; Alexander J. Federation¹; William E. Fondrie¹; ¹Talus Bioscience, Seattle, WA
- MOG am 09:30 **Investigating the limitations of (open) modification search engines for proteomics DIA data;** Robbin Bouwmeester¹; Robbe Devreese¹; Arthur Declercq¹; Alireza Nameni¹; Sven Degroove²; Kevin Velghe¹; Ralf Gabriels¹; Bart Van Puyvelde³; Sigrid Verhelst³; Maarten Dhaenens³; Lennart Martens¹; ¹VIB-UGent Center for Medical Biotechnology, Ghent, Belgium; ²VIB-UGent Center for Medical Biotechnology, Ghent, Belgium; ³Ghent University, Ghent, Belgium
- MOG am 09:50 **IsoPS-DIA: Dual Functionality of Targeted Quantification and Global Proteome Profiling;** Huan-Chi Chiu¹; Hsin-Ju Chan¹; Li-Yu Chen¹; Hsiang-En Hsu¹; Yu-Ju Chen^{1,2}; ¹Academia Sinica, Institute of Chemistry, Nankang, Taipei, Taiwan; ²National Taiwan University, Taipei City, Taiwan
- MOG am 10:10 **Simultaneous targeted and discovery-driven clinical proteotyping using hybrid-PRM/DIA;** Sandra Goetze^{1,2}; Audrey Van Drogen^{2,3}; Jonas B. Albinus³; Kyle L. Fort⁴; Tejas Gandhi⁵; Damiano Robbiani⁶; Véronique Laforte⁶; Lukas Reiter⁶; Mitchell P. Levesque⁶; Yue Xuan⁴; Bernd Wollscheid³; ¹ETHZ, Zurich, Switzerland; ²ETH PHRT Swiss Multi-Omics Center, Zurich, Switzerland; ³ETH Zurich, Zurich, Switzerland; ⁴Thermo Fisher Scientific, Bremen, Germany; ⁵Biognosys AG, Schlieren, Switzerland; ⁶University Hospital Zurich, Zurich, Switzerland

MOH am: Protein-Ligand and Protein-Protein Interactions Room 303ABCD (Level 3)

Session Chair: Ani Sahasrabudhe (Amgen)

- MOH am 08:30 **Establishing a native MS method to discover and track the 'glueing' of protein-protein interactions;** Danielle F. Kay¹; Carlo JA Verhoef²; Lars Van Dijk²; Richard G. Doveston³; Luc Brunsveld²; Peter J. Cossar²; Aneika C. Loney¹; ¹School of Biosciences, University of Birmingham, Birmingham, United Kingdom; ²Department of Biomedical Engineering and Institute for Complex Molecular Systems, Eindhoven University of Technology, Eindhoven, Netherlands; ³Leicester Institute of Structural and Chemical Biology and School of Chemistry, University of Leicester, Leicester, United Kingdom
- MOH am 08:50 **Elucidating HLTF-Mediated DNA Fork Remodeling via Native Mass Spectrometry;** Guan-Ting Lian^{1,2,3}; Yi-An Chen¹; Hui Emmanuela Miriam^{2,3,4}; Yi-Zhen Jiang³; Yen-Ju Chen³; Peter Chi^{3,5}; Hsin-Yung Yen⁵; ¹Institute of Biological Chemistry, Academia Sinica, Taipei city, Taiwan; ²Chemical Biology and Molecular Biophysics Program, Taiwan International Graduate Program, Academia Sinica, Taipei city, Taiwan; ³Institute of Biochemical Sciences, National Taiwan University, Taipei city, Taiwan; ⁴Institute of Molecular and Cellular Biology & Department of Medical Science, National Tsing Hua University, Hsinchu City, Taiwan; ⁵Institute of Biological Chemistry, Academia Sinica, Taipei city, Taiwan
- MOH am 09:10 **High-throughput protein-ligand analysis and targeted deconvolution enables identification of binders to intractable membrane proteins;** Konstantin Nagornov¹; Fernando Almeida²; Anton Kozhinov¹; Idir Liko²; Yury Tsybin¹; ¹Spectroswiss, Lausanne, Switzerland; ²OMass Therapeutics, Oxford, United Kingdom

MONDAY ORALS

- MOH am 09:30 **Structural dynamics and stability of membrane proteins interacting with lipids probed by native top-down mass spectrometry;** Jessie Le¹; Mark Arbing¹; Pascal Egea¹; Rachel Loo¹; Joseph Loo¹; ¹University of California, Los Angeles, Los Angeles, CA
- MOH am 09:50 **Probing molecular interactions of Bordetella pertussis Prn-1antigen with therapeutic monoclonal antibodies using native MS and complementary biophysical techniques;** Mohamed Ibrahim Gadallah¹; Virginia K James¹; Kate McConnell¹; Annalee W. Nguyen¹; Jennifer A. Maynard¹; Jennifer S. Brodbelt¹; ¹University of Texas at Austin, Austin, TX
- MOH am 10:10 **Unraveling Interactome Dynamics and Protein Function through Proteome-scale AP-MS Interaction Mapping and Structural Prediction;** Edward L. Huttlin¹; Laura Pontano Vaites¹; Sanjukta Guha Thakurta¹; Nathan Zuniga Pina¹; Lana D'Addieco¹; Austin Fergusson¹; Fana Gebreab¹; Emily Hill¹; Karina Martinez Perez¹; Nathan Bulloch¹; David Vanderwall¹; Ramin Rad¹; Sherry Liu¹; Joao A. Paulo¹; David Nusinow²; Donald S Kirkpatrick²; Tyrone Lee¹; Ludwig Geistlinger¹; Robert Gentleman¹; J Wade Harper¹; Steve Gygi¹; ¹Harvard Medical School, Boston, MA; ²Orion Medicines, San Francisco, CA
- Senescence - SKINMAGINE, Vienna, Austria; ³Medical University of Vienna, Vienna, Austria; ⁴Chanel PB, Pantin, France
- MOA pm 03:50 **Mapping the molecular landscape of 9p21 loss in bladder cancer through metabolic imaging;** Meredith L. Spradlin¹; Jianfeng Chen²; Bjoern Burckhardt³; Jianjun Gao²; Livia S. Eberlin³; ¹The University of Texas at Austin, Austin, TX; ²MD Anderson Cancer Center, Houston, Texas; ³Baylor College of Medicine, Houston, Texas
- MOA pm 04:10 **Pixelated Insights: Illuminating the Impact of Small Parasites on Host Metabolism through High-Resolution Mass Spectrometry Imaging;** Katja R Wiedemann¹; David Luh¹; Stefanie Gerbig²; Parviz Ghezellou¹; Alejandra Pilgram¹; Sven Heiles^{3, 4}; Martin Roderfeld⁵; Elke Roeb⁵; Christoph G Grevelding⁶; Liliana M R Silva⁶; Carlos Hermosilla⁶; Anja Taubert⁶; Kerstin Strupat⁷; Bernhard Spengler^{1, 2}; ¹Institute of Inorganic and Analytical Chemistry, Justus Liebig University, Giessen, Germany; ²Transmit GmbH, Giessen, Germany; ³Leibniz-Institut für Analytische Wissenschaften-ISIS-e.V., Dortmund, Germany; ⁴Faculty of Chemistry, University of Duisburg-Essen, Essen, Germany; ⁵Gastroenterology, Justus Liebig University, Giessen, Germany; ⁶Institute of Parasitology, Justus Liebig University, Giessen, Germany; ⁷Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- MOA pm: Imaging: Pharmaceuticals, Metabolites, Lipids, and Glycans**
Room 210ABC (Level 2)
 Session Chair: Jeffrey Spraggins (Vanderbilt University)
- MOB pm: Forensics: Innovations and Applications**
Room 207ABC (Level 2)
 Session Chair: Weihua Ji (National Institute of Standards & Technology (NIST))
- MOA pm 02:30 **Multimodal MALDI-MSI and hyperspectral microscopy reveals lipidomic changes during bronchopulmonary dysplasia;** Brittney L Gorman¹; Zhi Li²; Jeremy Clair¹; Gloria S Pryhuber³; Lingyan Shi²; Christopher R Anderton¹; ¹Pacific Northwest National Lab, Richland, WA; ²Shu Chien-Geno Lay Department of Bioengineering, University of California San Diego, San Diego, CA; ³Department of Pediatrics, University of Rochester Medical Center, Rochester, NY
- MOA pm 02:50 **DESI Imaging Mass Spectrometry reveals spatial changes of lipids in healthy and Alzheimer's mouse brains;** Artur Lazarian¹; Jason Mares²; Nicholas Bartelo³; Ana Paula Costa¹; Krista Wartchow¹; William Dartora¹; Tal Nuriel⁴; Jan Krumsiek³; Vilas Menon²; Laura Beth McIntire^{1, 4}; ¹Weill Cornell Medicine, New York, NY; ²Taub Institute for Research on Alzheimer's Disease and the Aging Brain, Department of Neurology, Columbia University Medical Center, New York, NY; ³Department of Physiology and Biophysics, Institute for Computational Biomedicine, Englander Institute for Precision Medicine, Weill Cornell Medicine, New York, NY; ⁴Department of Pathology and Cell Biology, Columbia University Medical Center, New York, NY
- MOA pm 03:10 **Quantitative Mass Spectrometry Imaging of Liposomal Doxorubicin Delivery and Bilayer Fate in Three-Dimensional Tumor Models;** Arbil Lopez¹; Joseph H Holbrook¹; Jessica Lukowski²; William Temple Andrews³; Gabrielle E Kemper¹; Amanda B Hummon¹; ¹The Ohio State University, Columbus, OH; ²Washington University School of Medicine, Saint Louis, MO; ³University of Maryland, Baltimore, Baltimore, MD
- MOA pm 03:30 **Exploring Cellular Senescence and Molecular Changes in Skin Aging with a Special Focus on N-glycosylation;** Samuele Zoratto^{1, 2}; Ralf Haider^{1, 2}; Christopher Kremslehner^{2, 3}; Gaëlle Gendronneau^{2, 4}; Florian Gruber^{2, 3}; Martina Marchetti-Deschmann^{1, 2}; ¹TU Wien, Vienna, Austria; ²Christian Doppler Laboratory for Multimodal Imaging of Aging and
- MOB pm 02:30 **Towards Isomeric Discrimination of Fentanyl by Energy-Resolved Mass Spectrometry;** Mark Dreyer¹; Brian Mayer²; ¹Forensic Science Center, Lawrence Livermore National Laboratory, Livermore, CA; ²Forensic Science Center, Lawrence Livermore National Laboratory, Livermore, CA
- MOB pm 02:50 **Eggs-amination of Volatiles Emissions of Blow Fly Eggs—Implications for Lucilia sericata Egg Age Estimation and Post Mortem Interval Determination;** Rabi A Musah¹; Alexa Figueroa¹; Jennifer Y. Rosati²; ¹University at Albany-SUNY, Albany, NY; ²John Jay College of Criminal Justice-CUNY, New York, NY
- MOB pm 03:10 **Rapid high-throughput screening of prohibited substances by coated blade spray-mass spectrometry for doping control;** Wei Zhou¹; JANUSZ PAWLISZYN¹; ¹University of Waterloo, Waterloo, ON
- MOB pm 03:30 **High-resolution and isotope ratio mass spectrometrybased profiling of Ricinus communis- A forensic approach;** Lisa Scharrenbroch^{1, 2}; Nicole Scheid¹; Thomas Holdermann¹; Thomas Schaefer¹; Björn Ahrens¹; Frederik Lermyte²; ¹Federal Criminal Police Office, Forensic Institute, Wiesbaden, Germany; ²Technical University of Darmstadt, Department of Chemistry, Darmstadt, Germany
- MOB pm 03:50 **Improved LCMS detection of opioids, amphetamines, psychedelics, and metabolites using TrEnDi;** Christian A Rosales¹; Noah A Lepinsky¹; Wondewossen Gebeyehu¹; Karl V Wasslen^{1, 2}; Benjamin B Warnes¹; Jasmine Chihabi¹; Jeffrey M Manthorpe^{1, 2}; Jeffrey C. Smith^{1, 2}; ¹Carleton University, Ottawa, ON; ²Carleton Mass Spectrometry Centre, Carleton University, Ottawa, ON
- MOB pm 04:10 **Quantitation of an Oral Fluid Drug Panel Including THC Using with High Resolution Accurate-Mass (HRAM) Mass Spectrometry;** Courtney Patterson¹; Kerry Hassell¹; ¹Thermo Fisher Scientific, San Jose, CA

MONDAY ORALS

MOC pm: Fundamentals: Unconventional Approaches in MS Room 304AB (Level 3)

Session Chair: Michael Glocker (Proteome Center Rostock)

- MOC pm 02:30 **Breaking chiral symmetry by directional rotation of ions in an ion trap;** Xiaoyu Zhou¹; Zhuofan Wang¹; Shuai Li¹; Xianle Rong¹; Jiexun Bu²; Qiang Liu¹; Zheng Ouyang¹; ¹Tsinghua University, Beijing, China; ²PURSPEC Technology (Beijing) Ltd., Beijing, China
- MOC pm 02:50 **Electric-field-free Approach to Ion Manipulation Based on Acoustic Fields;** Julia L Danischewski¹; Yi You²; Jens Riedel²; Jacob T Shelley¹; ¹Rensselaer Polytechnic Institute, Troy, NY; ²Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany
- MOC pm 03:10 **Development of a Forced Damped Harmonic Oscillator Model for the Characterization of Ion Parking of Native Protein Complexes;** Nicolas J Pizzala¹; Ian J Carrick¹; Jay S Bhanot¹; Eric T Dziekonski¹; Scott A McLuckey¹; ¹Purdue University, West Lafayette, IN
- MOC pm 03:30 **Using Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) to investigate Albumin Corona Formation on Chromium Oxide Nanoparticles;** Zoltan W Richter-Bisson¹; Heng-Yong Nie^{1, 2}; Yolanda Hedberg^{1, 2}; ¹Western University, London, ON; ²Surface Science Western, London, ON
- MOC pm 03:50 **Characterization of Lipid-Binding to Antimicrobial Peptides using Energy-variable Collision Induced Dissociation and Ultraviolet Photodissociation;** Jessica Hellinger¹; Justin Randall¹; Bryan Davies¹; Jennifer S. Brodbelt¹; ¹University of Texas - Austin, Austin, TX
- MOC pm 04:10 **High Energy Collision-induced Fragment Ions Simplify the LC/MS Detection of Heterogeneous Isoleuglandin-modified Autoantigens in Proteomic Analyses;** Daniel Roeth¹; Nathaniel Bloodworth²; David G Harrison²; Markus Kalkum¹; ¹City of Hope, Duarte, CA; ²Vanderbilt University, Nashville, TN

MOD pm: Environmental: Innovative Approaches and Instrumentation Room 304CD (Level 3)

Session Chair: Kaylie Kirkwood Donelson (National Institute of Environmental Health Sciences)

- MOD pm 02:30 **Novel ship-based and submersible Membrane Inlet-Photo-Ionization Mass Spectrometer (MI-PIMS) for on-line detection of environmental pollutants and explosives in sea water;** Sven Ehlert¹; Christian Gehm^{2,3}; Detlef Schulz-Bull³; Denis Starostin-Penner^{1, 2}; Carolin Schwarz²; Thorsten Streibel^{2, 4}; Andreas Walte¹; Norbert Graf⁵; Dorothee Niethammer⁵; Christian Menhard⁵; Eric Achterberg⁶; Björn Raupers⁶; Johannes Passig^{2, 4}; Ralf Zimmermann^{2, 4}; ¹Photonion GmbH, Schwerin, Germany; ²University of Rostock, Rostock, Germany; ³Leibniz Institute of Baltic Sea Research (IOW), Rostock, Germany; ⁴Joint Mass Spectrometry Centre, Cooperation Group "Comprehensive Molecular Analytics" (CMA), Helmholtz Munich, Munich, Germany; ⁵InnoLas Laser GmbH, Krailing, Germany; ⁶GEOMAR Helmholtz Centre for Ocean Research Kiel, Kiel, Germany
- MOD pm 02:50 **Chemical Characterization of Polymer Content in Plastic Materials Using Pyrolysis - Direct Analysis in Real Time - High-Resolution Mass Spectrometry;** Emily R Halpern¹; Peter Christ²; Killian MacFeely²; Lauren Heirly²; Christopher West²; Yitao Li³; Won Kim⁴; Anthony Mennito⁴; Alexander Laskin²; ¹Purdue University, West Lafayette, IN; ²Purdue University, Department of Chemistry, West Lafayette, IN; ³Purdue University, Department of

Statistics, West Lafayette, IN; ⁴Exxon Mobil, Annandale, NJ

- MOD pm 03:10 **Novel LC Separation for Comprehensive Analysis of Net-Zero Bio-oils by Ultra-High-Resolution Mass Spectrometry;** Martha Liliana Chacon-Patino¹; Joseph W Frye-Jones¹; Lissa C. Anderson¹; David C. Dayton²; Pierre Giusti³; Alvaro J Tello-Rodriguez¹; Germain Salvato Vallverdu⁴; Christopher Rüger⁵; Caroline Barrère-Mangote³; Christopher L Hendrickson¹; Brice Bouyssiere⁴; Carlos Afonso⁶; Christopher Holder Montenegro¹; Ryan P Rodgers¹; ¹National High Magnetic Field Laboratory, Tallahassee, Florida; ²RTI International, Technology Advancement and Commercialization, Research Triangle Park, NC; ³TotalEnergies, Harfleur, France; ⁴University of Pau and the Adour Region, Pau, France; ⁵University of Rostock, Rostock, Germany; ⁶University of Rouen-Normandy, Mont-Saint-Aignan, France
- MOD pm 03:30 **Rapid Detection of Per- and Polyfluoroalkyl Substances (PFAS) Using Paper Spray-Based Mass Spectrometry;** Md. Tanim-Al Hassan¹; Praneeth Ivan Joel FNU¹; Hao Chen¹; ¹New Jersey Institute of Technology, Newark, NJ
- MOD pm 03:50 **Guarding drinking water safety against harmful algal blooms: Could UV/ Cl2 treatment be the answer?;** Susan Richardson¹; Alexandria Forster¹; Patrick T Justen¹; Minghao Kong²; Dionysios Dionysiou²; ¹University of South Carolina, Columbia, SC; ²University of Cincinnati, Cincinnati, OH
- MOD pm 04:10 **Metabolomics of urine gathered from wilderness snow correlates with nutritional status of wild moose, Alces alces, on Isle Royale, Michigan;** James Bain¹; Sarah Hoy²; Leah M Vucetich²; Rolf Peterson²; John A Vucetich²; Stephan Baumann³; Natalie Rasmussen³; Daniel Cuthbertson³; Michael J Muehlbauer¹; Madison Strain¹; David E Lee¹; Demitrius Hill¹; Ky Koitzsch²; Lisa O Koitzsch²; ¹Duke University, Durham, NC; ²Michigan Technological University, Houghton, MI; ³Agilent Technologies, Santa Clara, CA

MOE pm: Instrumentation: Innovative Separation Approaches Coupled to MS (In Memory of Andy Alpert) Ballroom DE (Level 3)

Session Chair: Jake Melby (AstraZeneca)

- MOE pm 02:30 **Revealing Unseen Glycans with HILIC-HRIMS-MS;** Ron Orlando¹; Hoang Kim Ngan Thai¹; ¹University of Georgia, Athens, GA
- MOE pm 02:50 **Hydrophilic interaction chromatography coupled to ultraviolet photodissociation affords identification, localization, and relative quantitation of glycans on intact glycoproteins;** Virginia K James¹; Annika A.M. Van Der Zon²; Edwin E. Escobar¹; Andrea F. G. Gargano²; Jennifer S. Brodbelt¹; ¹The University of Texas at Austin, Austin, TX; ²The University of Amsterdam, Amsterdam, Netherlands
- MOE pm 03:10 **Rapid Intact Protein Quantification and Identification using IEX for Novel Biodesigned Proteins;** Mathew Ellenberger¹; Anastasia Lindahl¹; ¹Geltor, Emeryville, CA
- MOE pm 03:30 **Removal of artifacts from Hadamard transform multiplexing of online SEC with CD-MS;** October N Owen¹; James D. Sanders¹; Michael Thomas Marty¹; ¹University of Arizona, Tucson, AZ
- MOE pm 03:50 **Assay screening and target isolation workflows hyphenated to MS for analysis and characterization of (bio)pharmaceuticals in industrial settings;** Rodell Barrientos¹; Gioacchino L Losacco¹; Heather Wang¹; Andrew Singh¹; Imad A Haidar Ahmad¹; Emmanuel Appiah-Amponsah¹; Erik Regalado¹; ¹Analytical Research and Development, Merck & Co., Inc., Rahway, NJ

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MOE pm 04:10 **SPE-CZE-MS using Orbitrap Astral for high-throughput phosphoproteomics analyses from limited sample amounts;** [Lia Serrano](#)¹; Joshua J Coon^{2, 3}; Scott J Mellors⁴; J. Will Thompson⁴; ¹University of Wisconsin Madison, Madison, WI; ²University of Wisconsin-Madison, Madison, WI; ³Morgridge Institute for Research, Madison, WI; ⁴908 Devices Inc., Boston, MA

MOF pm: Lipidomics: Targeted and Untargeted Ballroom C (Level 3)

Session Chair: [Jace Jones](#) (University of Maryland)

MOF pm 02:30 **Semi-quantification of triglycerides with resolved fatty acid composition using a targeted MS3 approach on a novel hybrid nominal mass instrument;** [Hector Gallart-Ayala](#)¹; Julijana Ivanisevic¹; Charles Maxey^{2, 3}; Rahul Deshpande²; Bashar Amer³; Susan S Bird³; Philip M. Remes³; Claudia P.B. Martins³; Cristina C. Jacob³; ¹University of Lausanne, Lausanne, Switzerland; ²ThermoFisher Scientific, San Jose, CA; ³Thermo Fisher Scientific, San Jose, CA

MOF pm 02:50 **Advancing Absolute Lipid Quantification in Nontargeted LC-HRMS/MS Analysis by Multi-Point Calibration;** [Lauren Bishop](#)¹; Oliver Fiehn¹; ¹University of California, Davis, Davis, California

MOF pm 03:10 **Isobaric Labeling of Multiple Lipid Classes toward Multiplexed LC-MS/MS-based Quantitative Analysis;** [Shuling Xu](#)¹; Zhijun Zhu¹; Zicong Wang¹; Peng-Kai Liu¹; Yuan Liu¹; Gaoyuan Lu¹; Michael Rigby¹; Luigi Puglielli¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI

MOF pm 03:30 **Comprehensive discovery lipidomic workflow which utilizes a novel, multi-reflecting ToF with integrated informatics, providing highly confident lipid characterization and quantification;** [Nyasha C Munjoma](#)¹; Jayne Kirk¹; Lee A Gethings¹; Paolo Tiberi²; Laura Goracci³; Richard Lock¹; ¹Waters Corporation, Wilmslow, United Kingdom; ²Mass Analytica Ltd, Sant Cugat del Vallés, Spain; ³University of Perugia, Perugia, Italy

MOF pm 03:50 **Untargeted 2DxLC-Mass Spectrometry Workflow using CID and EAD for the Quantification and Comprehensive Structural Characterization of Glycerophospholipids in Plasma Samples;** [Laura Gisela González Iglesias](#)¹; Renzo Picononi²; Guenter Boehm²; Gerard Hopfgartner¹; ¹LSMS, Department of Inorganic and Analytical Chemistry, University of Geneva, Geneva, Switzerland; ²CTC Analytics AG, Zwingen, Switzerland

MOF pm 04:10 **Lipidomics highlights the role of fatty acids in cell survival and death in the presence of cholesterol dysregulation;** [Ralph John Emerson Javier Molino](#)¹; Stephanie M Cologna^{1, 2}; Mark Schultz³; Olivia Klein³; ¹Department of Chemistry, University of Illinois Chicago, Chicago, Illinois; ²Laboratory of Integrated Neuroscience, University of Illinois Chicago, Chicago, Illinois; ³Stead Family Department of Pediatrics, Carver College of Medicine, University of Iowa, Iowa City, IA

MOG pm: Biotherapeutics: Proteins, Antibodies, and Antibody/Drug Conjugates Ballroom AB (Level 3)

Session Chair: [Richard Y.-C. Huang](#) (Johnson & Johnson Innovative Medicine)

MOG pm 02:30 **Utilizing Mass Spectrometry to Overcome Challenges in Unveiling Molecular Identity of Emerging Biotherapeutics;** Thierry Besson¹; Jennifer Kang²; Daniela Miranda¹; Sebastien Ripoché¹; Hon-Ren Huang²; [Patrick Schindler](#)¹; ¹Novartis, Basel, Switzerland; ²Novartis, Cambridge, MA

MOG pm 02:50 **Characterizing Antibody/Drug Conjugates by Coupling The SampleStream Platform and**

Newomics' MnESI Source with Charge Detection Mass Spectrometry; Keely Fuller¹; Phillip Chu²; Cheng-Wei Jeff Lin³; Lizzie Harmon²; Daojing Wang⁴; Philip D. Compton⁵; Jared Kafader⁶; Jonathan L Josephs²; John C Tran²; [Rachel Shi](#)²; ¹Genentech, South San Francisco, CA; ²Genentech Inc., South San Francisco, CA; ³Genentech, Inc., South San Francisco, CA; ⁴Newomics Inc., Berkeley, CA; ⁵Integrated Protein Technologies, Inc, Evanston, IL; ⁶Northwestern University, Chicago, IL

MOG pm 03:10 **Investigating the impact of small-molecule conjugation location on mAb stability and structure using ion mobility-mass spectrometry and collision induced unfolding;** [Nicole A Rivera-Fuentes](#)¹; Addison E. Bergman¹; Vanessa Quevedo-Barrios¹; Brandon T Ruotolo¹; ¹University of Michigan Department of Chemistry, Ann Arbor, MI

MOG pm 03:30 **Evaluating Stress-Induced Structural Changes in Antibodies via Surface Induced Dissociation and Gas Phase Unfolding;** [Rowan Matney](#)¹; Eledon Beyene¹; Varun V Gadkari¹; ¹University of Minnesota, Minneapolis, MN

MOG pm 03:50 **Automated Real Time High-Speed Microdroplet Reactions to Increase the Throughput of Therapeutic Protein Characterization;** [Krishna Anapindi](#)¹; Edward J. Hsieh¹; Jim Lau²; Daniela M. Tomazela³; ¹Gilead Sciences, Foster City, CA; ²Agilent Technologies, Santa Clara, CA; ³Gilead Sciences Inc., Foster City, CA

MOG pm 04:10 **Proteform specific microheterogeneity assessment of biopharmaceuticals using a modified Orbitrap Tribrid mass spectrometer;** Corentin Beaumal¹; Kristina Srzentic²; Sara Carillo¹; Florian Füssli¹; Silvia Millan Martin¹; Andrew Norris²; Rafael Melani³; [Jonathan Bones](#)^{1, 4}; ¹The National Institute for Bioprocessing Research & Training, Dublin, Ireland; ²Thermo Fisher Scientific, Reinach, Switzerland; ³Thermo Fisher Scientific, San Jose, CA; ⁴School of Chemical and Bioprocess Engineering, University College Dublin, Belfield, Ireland

MOH pm: Informatics: Innovations Room 303ABCD (Level 3)

Session Chair: [Susan Weintraub](#) (University of Texas San Antonio Health Science Center)

MOH pm 02:30 **MS_Draw: A New Software Tool for Annotating High-Resolution Mass Spectra of Organic Compounds;** [Xiaoyu Yang](#)¹; Pedatsur Neta¹; H. Martin Garraffo¹; Dmitrii V Tchekhovskoi¹; Yuri A Mirokhin¹; Stephen E Stein¹; ¹NIST, Gaithersburg, MD

MOH pm 02:50 **Massbild: A Streamlined Informatic Workflow for Identification and Visualization of Proteoforms in Imaging Mass Spectrometry;** [Indira Pla](#)¹; Michael A.R. Hollas¹; Bryan P. Early¹; Pei Su¹; Nathaniel Henning^{1, 2}; Vijaya Lakshmi Kanchustambham¹; Michael A. Caldwell¹; Ryan T. Fellers¹; Neil L. Kelleher¹; ¹Proteomics Center of Excellence, Northwestern University, Evanston, Illinois; ²Chemistry of Life Processes Institute, Northwestern University, Evanston, IL

MOH pm 03:10 **Keep your friends close: Neighborhood based clustering for feature extraction in diaPASEF data;** [Juan Sebastian S Paez](#)¹; Andrea I Gutierrez¹; Daniele Canzani¹; Alexander J Federation¹; Lindsay K Pino¹; William E Fondrie¹; ¹Talus Bioscience, Seattle, WA

MOH pm 03:30 **Deep learning-driven de novo peptide sequencing of post-translationally modified and unmodified peptides;** [Daniela Klaproth-Andrade](#)¹; Johannes Hingerl¹; Yanik Bruns¹; Nicholas Smith¹; Mathias Wilhelm²; Julien Gagneur¹; ¹Technical University of Munich, Garching bei Muenchen,

MONDAY ORALS

- Germany; ²Technical University of Munich, Freising, Germany
- MOH pm 03:50 Deep Learning Enables Targeted Proteomics With Sample Multiplexing Without PRM Scheduling, Synthetic Peptides, or Data Libraries; Steven Shuken¹; Edward L. Huttlin¹; Qing Yu¹; Steven P. Gygi¹; ¹Department of Cell Biology, Harvard Medical School, Boston, MA
- MOH pm 04:10 **PASTAQ: threshold avoiding LC-MS(/MS) data pre-processing for untargeted proteomics and metabolomics profiling**; Alejandro Sánchez Brotons¹; Jonatan Eriksson²; Marcel Kwiatkowski³; Justina Wolters⁴; Ido Kema⁴; Andrei Barcaru¹; Folkert Kuipers⁴; Stephan Bakker⁴; Rainer Bischoff¹; Frank Suits⁵; Peter Horvatovich¹; ¹University of Groningen, Groningen, Netherlands; ²Lund University, Lund, Sweden; ³University of Innsbruck, Innsbruck, Austria; ⁴University Medical Center Groningen, Groningen, Netherlands; ⁵IBM Australia, Melbourne, Australia

TUESDAY ORALS

TOA am: Imaging: Instrumentation & Method Development Room 210ABC (Level 2)

Session Chair: Josephine Bunch (National Physical Laboratory)

- TOA am 08:30 **Histology-Guided Single-Cell Mass Spectrometry Imaging of Tissue and Cell Culture Using a Transmission-mode MALDI-2 Ion Source with Integrated Fluorescence Microscopy;** Jens Soltwisch¹; Alexander Potthoff¹; Marcel Niehaus²; Sebastian Bessler¹; Jan Schwenzfeier¹; Jens Hoehndorf²; Klaus Dreisewerd¹; ¹*Institute of Hygiene, University of Münster, Münster, Germany*; ²*Bruker Daltonics GmbH & Co.KG, Bremen, Germany*
- TOA am 08:50 **Deep MALDI-MS Spatial 'Omics in Mouse Kidney and Human Biculture Cancer Spheroids Guided by Quantum Cascade Laser Mid-infrared Imaging Microscopy;** Lars Gruber^{1, 2}; Stefan Schmidt¹; Stefania A. Iakab¹; Enzlein Thomas¹; Huong Giang Vo³; James L. Cairns^{1, 2}; Yasemin Furtun Ucal¹; Florian Keller¹; Denis Abu Sammour¹; Rüdiger Rudolf¹; Matthias Eckhardt⁴; Laura Bindila³; Carsten Hopf^{1, 2, 5}; ¹*CeMOS, Bioanalytics, University of Applied Sciences Mannheim, Mannheim, Germany*; ²*Heidelberg University, Medical Faculty, Heidelberg, Germany*; ³*Clinical Lipidomics Unit, Institute of Physiological Chemistry, University of Medical Center of the JGU Uni Mainz, Mainz, Germany*; ⁴*Institute of Biochemistry and Molecular Biology, University of Bonn, Bonn, Germany, Bonn, Germany*; ⁵*Mannheim Center for Translational Neuroscience (MCTN), Mannheim, Germany*
- TOA am 09:10 **Mid-infrared picosecond laser assisted LD-REIMS imaging towards single cell resolution;** Yu Wang¹; Ronan Battle¹; Daniel Simon^{1, 2}; Yuchen Xiang¹; Samuel Azevedo Magalhães¹; Kenneth Robinson^{1, 2}; Stefania Maneta-Stavarakaki¹; Timothy Runcorn¹; Zoltan Takats^{1, 2}; Robert Murray¹; ¹*Imperial College London, London, United Kingdom*; ²*Rosalind Franklin Institute, Didcot, United Kingdom*
- TOA am 09:30 **Multi-Site Reproducibility Trial of MALDI-IHC Multiplexed Targeted Protein Imaging using a 33-Organ Tissue Microarray;** Catelynn C Shafer¹; Joseph H Holbrook²; Catherine A Kita³; Gargey B. Yagnik³; Mark J. Lim³; Kenneth J. Rothschild^{3, 4}; Katherine A. Stump⁵; Erin H. Seeley⁶; Elizabeth K Neumann⁷; Amanda B. Hummon⁸; ¹*University of California Davis, Davis, CA*; ²*Ohio State University, Columbus, OH*; ³*AmberGen Inc., Billerica, MA*; ⁴*Boston University, Department of Physics and Photonics Center, Boston, MA*; ⁵*Bruker Daltonics GmbH & Co. KG, Billerica, MA*; ⁶*University of Texas - Austin, Austin, TX*; ⁷*University of California, Davis, Davis, California*; ⁸*The Ohio State University, Columbus, OH*
- TOA am 09:50 **High resolution low flow DESI imaging using a commercial DESI source;** Mark Towers¹; Alex Birsan²; Emrys Jones³; Joanne Ballantyne¹; Sheba Jarvis⁴; ¹*Waters Corporation, Wilmslow, United Kingdom*; ²*Waters, Milford, MA*; ³*Waters Corporation, Wilmslow, United Kingdom*; ⁴*Imperial College London, Hammersmith Hospital, London, United Kingdom*
- TOA am 10:10 **Native nano-DESI mass spectrometry imaging of proteins of up to 230 kDa – A twofold improvement in molecular weight;** Oliver Hale¹; Rosa Viner²; Weijing Liu²; Rafael Melani²; Christopher Mullen²; Helen Cooper¹; ¹*School of Biosciences, University of Birmingham, Birmingham, United Kingdom*; ²*Thermo Fisher Scientific, San Jose, CA*

TOB am: Small Molecules: Structural Characterization and Quantification Room 207ABC (Level 2)

Session Chair: Tobias Kind (Enveda Biosciences)

- TOB am 08:30 **Shedding light on the dark metabolome: Structural identification of three novel metabolites using chemical tagging and tandem MS;** Julius Agongo¹; Scott Grady¹; Kevin Cho²; Benjamin Bythell³; Gary Patti²; Christopher Arnatt¹; James Edwards¹; ¹*Saint Louis University, Saint Louis, MO*; ²*Washington University in Saint Louis, St. Louis, MO*; ³*Ohio State University, Columbus, OH*
- TOB am 08:50 **Distinguishing isomeric saccharides and saccharide-derivatives using far-infrared ion spectroscopy;** Rianne E. Van Outersterp¹; Moritz Rahm¹; Pieter C. Kooijman²; Jona Merx³; Udo F. H. Engelke⁴; Mei-Lan H. Tonnejck²; Kas J. Houthuijs²; Giel Berden²; Tessa M. A. Peters⁴; Michel A. A. P. Willemsen⁵; Karlien L. M. Coene⁴; Ron A. Wevers⁴; Hans J. C. T. Wessels⁴; Thomas J. Boltje³; Jos Oomens²; Jonathan Martens²; Dirk J. Lefeber¹; ¹*Radboud Consortium for Glycoscience, Department of Neurology, Donders Institute for Brain, Cognition, and Behavior, Radboud University Medical Center, Nijmegen, Netherlands*; ²*Institute for Molecules and Materials, FELIX Laboratory, Radboud University, Nijmegen, Netherlands*; ³*Institute for Molecules and Materials, Radboud Consortium for Glycoscience, Synthetic Organic Chemistry, Radboud University, Nijmegen, Netherlands*; ⁴*Department of Human Genetics, Radboud Consortium for Glycoscience, Translational Metabolic Laboratory, Radboud Institute for Molecular Life Sciences, Radboud University Medical Center, Nijmegen, Netherlands*; ⁵*Amalia Children's Hospital, Department of Pediatric Neurology & Donders Institute for Brain, Cognition and Behaviour, Radboud University Medical Centre, Nijmegen, Netherlands*
- TOB am 09:10 **Rapid and specific determination of arginine and citrulline with library confirmation using a novel acoustic ejection HRMS;** Aaron Stella¹; Jacob W McCabe²; Anuja Bhalkikar²; Han Joo Lee²; ¹*SCIEX, Framingham, MA*; ²*Sciex, Framingham, MA*
- TOB am 09:30 **A Multidimensional Identification Strategy of Metabolites in Human Milk Using Spectral Libraries and Standard Reference Materials (SRM);** Aliyah Hannah A. Remoroza^{1, 2}; Yamil Simón-Manso¹; Meghan C Burke¹; Tytus Mak¹; Stephen E Stein¹; ¹*National Institute of Standards and Technology, Gaithersburg, MD*; ²*UMBC, Baltimore, MD*
- TOB am 09:50 **Benylation followed by LC-ESI-QTOFMS improves sensitivity for the analysis of low molecular weight organic acids in the rhizosphere;** Teresa Steininger-Mairinger¹; Pascal Stopper¹; Philipp Tondl¹; Alice Tognacchini¹; Markus Puschenreiter¹; Stephan Hann¹; Christina Troyer¹; ¹*University of Natural Resources and Life Sciences-BOKU Vienna, Vienna, Austria*
- TOB am 10:10 **A post-LC multi labeling approach to boost structure elucidation and confidence in non-targeted metabolomics;** Giovanni Andrea Vitale¹; Kai Dührkop²; Robin Schmid³; Sebastian Böcker²; Mingxun Wang⁴; Yvonne Mast⁵; Stephanie Grond¹; Heike Broetz-Oesterhelt¹; Chambers Connor Hughes¹; Daniel Petras^{1, 4}; ¹*University of Tuebingen, Interfaculty Institute of Microbiology and Infection Medicine, Tuebingen, Germany*; ²*Friedrich-Schiller-University, Jena, Germany*; ³*Institute of Organic Chemistry and Biochemistry of the CAS, Prague, Czech Republic*; ⁴*University of California, Riverside, Riverside, CA*; ⁵*Leibniz Institute DSMZ German Collection of Microorganisms and Cell Cultures, Braunschweig, Germany*

TOC am: Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, and Supplements Room 304AB (Level 3)

TUESDAY ORALS

Session Chair: Melanie Downs (University of Nebraska)

TOC am 08:30 **Investigating the Impact of Replicates for Different Food Matrices on Non-Targeted Analysis Results;** Karen E Butler¹; Erica Bakota²; Christine M Fisher¹; Ann M Knolhoff¹; ¹Center for Food Safety and Applied Nutrition, United States Food and Drug Administration, College park, Maryland; ²Kansas City Human and Animal Food Laboratory, United States Food and Drug Administration, Lenexa, Kansas

TOC am 08:50 **Untargeted characterization of short peptides in complex food matrices;** Marie YAMMINE^{1, 2}; Marc Haegelin¹; Fabrice Bray¹; Juliette Caron²; Christian ROLANDO¹; Isabelle Mouly²; ¹UAR CNRS 3290 - MSAP, Villeneuve d'ascq, France; ²Lesaffre Institute of Science and Technology, Lesaffre International, Marquette-Lez-Lille, France

TOC am 09:10 **Quantitative analysis of plant phenolics by LC-MS/MS, and PhenolicsDB: a publicly available high-resolution MS/MS spectral library;** Cristian Daniel Quiroz-Moreno¹; Jessica L Cooperstone¹; ¹Ohio State University, Columbus, OH

TOC am 09:30 **Quantification of intact staphylococcal enterotoxin A and variants by top-down mass spectrometry in dairy products in the low ng/mL range;** Nina Aveilla^{1, 2}; Cécile Féraudet-Tarisse¹; Abdelhak Fatih²; Jacques-Antoine Hennekinne²; Yacine Nia²; François Fenaille¹; Stéphanie Simon¹; François Bécher¹; ¹Université Paris-Saclay, CEA, DRF, Département Médicaments et Technologies pour la Santé (DMTS), Service de Pharmacologie et d'Immunoanalyse (SPI), Gif-sur-Yvette, France; ²Laboratory for Food Safety, French Agency for Food, Environmental and Occupational Health & Safety (ANSES), Maisons-Alfort, France

TOC am 09:50 **Detection of Transgenic Proteins in Corn-Based Processed Foods Using Data-Independent Mass Spectrometry;** Stephen Swatkoski¹; Matthew Miele¹; ¹FDA/CFSAN, College Park, MD

TOC am 10:10 **Unveiling protein digestibility and prebiotic potential of bovine milk and plant-based alternatives via LC-MS/MS-based peptidomics and glycomics;** Yu-Ping Huang¹; Yu Wang¹; You-Tae Kim¹; Gulustan Ozturk²; Aidong Wang¹; Bruna Paviani¹; Naomi K. Fukagawa³; Katherine Phillips⁴; David A. Mills¹; Daniela Barile¹; ¹University of California, Davis, Davis, CA; ²University of Wisconsin-Madison, Madison, WI; ³USDA-ARS, Beltsville, MD; ⁴Virginia Tech, Blacksburg, Virginia

**TOD am: Synthetic Polymers
Room 304CD (Level 3)**

Session Chair: Scott Grayson (Tulane University)

TOD am 08:30 **Pyrolysis and Thermal Extraction of Polymeric Materials with Suction-driven, Real-time Chemical Ionization Sources and Rapid Polarity Switching;** G. Asher Newsome¹; Katja S. Diaz-Granados^{1, 2}; Joshua D. Caldwell²; Erin R. Birdsall^{1, 3}; ¹Smithsonian Museum Conservation Institute, Suitland, MD; ²Vanderbilt University, Nashville, TN; ³Smithsonian National Museum of the American Indian, Suitland, MD

TOD am 08:50 **Elucidating Gas-Phase Polymer and Denatured Protein Structures Using Ion Mobility-Tandem Mass Spectrometry: Insights from Experimental and Molecular Dynamics Analyses;** Levan Hua¹; Hailey Kaylor²; Carlos Larriba-Andaluz¹; ¹Indiana University Purdue University Indianapolis, Indianapolis, IN; ²Colorado School of Mines, Golden, CO

TOD am 09:10 **Structure and dynamics of insoluble bismuth oxide-based polymers using LDI MS and in situ isotope exchange;** Daniil G Ivanov¹; Chanbopha

Tho¹; Daniel Favre¹; Igor A. Kaltashov¹; ¹University of Massachusetts Amherst, Amherst, MA

TOD am 09:30 **Streamlining Pharmaceutical Polymer LC-MS Analysis by Fourier Transform-based Deconvolution and Macromolecular Mass Defect Analysis;** Andy Swansiger¹; Chris M Crittenden²; James Prell¹; Bifan Chen²; ¹University of Oregon, Eugene, OR; ²Genentech Inc., South San Francisco, CA

TOD am 09:50 **NP-SIMS as a tool for evaluating the homogeneity of extreme-ultraviolet resists and their performance;** Jander Cruz¹; Dmitriy Verkhoturov²; Stanislav Verkhoturov²; Emile Schweikert²; Michael Eller¹; ¹California State University Northridge, Northridge, CA; ²Texas A&M, College Station, TX

TOD am 10:10 **Probing the Reaction Mechanisms and Microstructures of Polyether Polyols and Their Associated Copolymers;** Anthony P Gies¹; David M Hercules²; ¹LYB, Cincinnati, OH; ²Vanderbilt University, Nashville, TN

**TOE am: Clinical Analysis: Innovations
Ballroom DE (Level 3)**

Session Chair: Kara Lynch (University of California, San Francisco)

TOE am 08:30 **Using Ion Mobility to Help Make Mass Spec Mainstream: A Case Study in Urine Toxicology;** Frederick Strathmann¹; Zongyuan Chen¹; Alan McKenzie-Coe¹; Miriam Fico¹; Joshua K McBee¹; Lauren Royer¹; Daniel DeBord¹; ¹MOBILion Systems, Chadds Ford, PA

TOE am 08:50 **Revisiting the MALDI MS in the clinical laboratories: A cornerstone for the new Clostridium difficile toxin activity detection method;** Josef Dvorak^{1, 2}; Petr Pompach^{2, 3}; Michael Volny⁴; Jaroslav Hrabak^{5, 6}; Petr Novak^{2, 7}; ¹Institute of Microbiology of the CAS, v. v. i., Prague, Czech Republic; ²Faculty of Science, Charles University, Prague, Czech Republic; ³Institute of Biotechnology CAS, Vestec, Czech Republic; ⁴University of Chemistry and Technology, Prague, Czech Republic; ⁵Biomedical Center, Faculty of Medicine, Charles University, Pilsen, Czech Republic; ⁶Department of Microbiology, Faculty of Medicine, Charles University, Pilsen, Czech Republic; ⁷Institute of Microbiology CAS, Prague, Czech Republic

TOE am 09:10 **Affinity MALDI chips for clinical and diagnostic applications: Possibilities and limitations for future medical devices;** Michael Volny^{1, 2, 3}; Petr Pompach^{2, 4}; Jana Novakova²; Josef Dvorak^{1, 5}; Zuzana Kalaninova^{1, 5}; Petr Novak¹; ¹Institute of Microbiology CAS, Prague, Czech Republic; ²AffiPro s.r.o, Vestec, Czech Republic; ³University of Chemistry and Technology Prague, Prague 6 - Dejvice, Czech Republic; ⁴Institute of Biotechnology CAS, Vestec, Czech Republic; ⁵Charles University, Prague 2, Czech Republic

TOE am 09:30 **Adapting the MasSpec Pen Technology for Minimally Invasive Mouth Cancer Screening;** Emily X. Ma¹; Charles A. Wolfe^{1, 2}; Michael F. Keating^{1, 2}; Gabrielle Wolter¹; Carlos Chone³; Erich M. Sturgis¹; Livia S. Eberlin¹; ¹Baylor College of Medicine, Houston, TX; ²University of Texas at Austin, Austin, TX; ³University of Campinas, Campinas, Brazil

TOE am 09:50 **Digging into the multifaceted variability of antibody molecules: Fc-proteoform profiling illuminates autoimmune responses in rheumatoid arthritis;** Constantin Blöchl¹; Eva Maria Stork²; Hans Ulrich Scherer²; Rene E. M. Toes²; Manfred Wuhrer¹; Elena Domínguez-Vega¹; ¹Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; ²Department of Rheumatology, Leiden University Medical Center, Leiden, Netherlands

TUESDAY ORALS

TOE am 10:10 **Changes in Protein Expression Following a STEMI in Diabetic Patients Treated with Sodium-Glucose Transport Protein 2 Inhibitors;** Megan ME Tomilin¹; Jay Shavadia¹; Gudrun Caspar-Bell¹; Paulos Chumala¹; Rama Mangipudi¹; Brooke Thompson¹; Haissam Haddad¹; George Katselis¹; ¹University of Saskatchewan, Saskatoon, SK

TOF am: Covalent Labeling and Chemical Crosslinking Ballroom C (Level 3)

Session Chair: Huilin Li (Sun Yat-sen University)

TOF am 08:30 **Don't Waste Time – Ensure Success in Your Cross-Linking Mass Spectrometry Experiments Before You Begin;** Lucienne Nouchikian^{1,2,3}; David Fernandez-Martinez^{2,4,5}; Pierre-Yves Renard^{6,7}; Cyrille Sabot^{6,7}; Guillaume Duménil^{2,4,5}; Martial Rey^{2,4,8}; Julia Chamot-Rooke^{2,4,8}; ¹Institut Pasteur, Paris, France; ²Université Paris Cité, Paris, France; ³CNRS UAR2024, Paris, France; ⁴Institut Pasteur, Paris, France; ⁵INSERM UMR1225, Paris, France; ⁶Univ Rouen Normandie, Rouen, France; ⁷COBRA UMR 6014, Rouen, France; ⁸CNRS UAR2024, Paris, France

TOF am 08:50 **Click-linking: achieving high in situ crosslinking efficiency by orthogonal 2-step-linking on fixed and stabilized cells;** Bruno C. Amaral¹; Andrew RM Michael¹; Nicholas Brodie¹; David C Schriemer¹; ¹University of Calgary, Calgary, AB

TOF am 09:10 **Quantitative glycan-protein cross-linking mass spectrometry reveals the role of glycan heterogeneity in protein-protein interaction networks;** Michael Russelle S. Alvarez¹; Siyu Chen¹; Yixuan Xie¹; Sheryl Joyce G. Alvarez¹; Anirudh Yadlapati¹; Shivraj Gill¹; Carlito B. Lebrilla¹; ¹University of California Davis, Davis, CA

TOF am 09:30 **Leveraging cross-linking mass spectrometry for modelling antibody-antigen complexes and potential strategy for antibody deimmunization;** Luca M. Barbero¹; Andrea Di Ianni²; Alessio Di Ianni³; Kyra Cowan⁴; Federico Riccardi-Sirtori¹; ¹RBM Merck, Colleretto Giacosa, Italy; ²University of Turin, Turin, Italy; ³University Halle-Wittenberg, Halle (Saale), Germany; ⁴Merck KGaA, Darmstadt, Germany

TOF am 09:50 **Trifluoromethylation Multiplex Chemical Labeling Enhances the Resolution of Hydroxyl Radical Protein Footprinting;** Rohit Jain¹; Erik Farquhar¹; Nanak S. Dhillon¹; Nayeon Jeon¹; Mark R Chance¹; Janna Kiselar¹; ¹Case Western Reserve University, Cleveland, OH

TOF am 10:10 **Radical Protein Footprinting in Mammalian Whole Blood;** Joshua S. Sharp¹; Lyle Tobin¹; Haolin Luo²; Sandeep K. Misra¹; Lisa M. Jones²; ¹University of Mississippi, University, MS; ²University of California San Diego, La Jolla, CA

TOG am: Top Down Protein and Proteoform Analysis Ballroom AB (Level 3)

Session Chair: Kellye Cupp-Sutton (University of Alabama)

TOG am 08:30 **Influence of Different Sample Preparation Approaches on Proteoform Identification by Top-Down Proteomics;** Philipp T. Kaulich¹; Kyowon Jeong^{2,3}; Oliver Kohlbacher^{2,3,4}; Andreas Tholey¹; ¹Systematic Proteome Research & Bioanalytics, Institute for Experimental Medicine, Christian-Albrechts-Universität zu Kiel, Kiel, Germany; ²Applied Bioinformatics, Department for Computer Science, University of Tübingen, Tübingen, Germany; ³Institute for Bioinformatics and Medical Informatics, University of Tübingen, Tübingen, Germany; ⁴Translational Bioinformatics, University Hospital Tübingen, Tübingen, Germany

TOG am 08:50 **Proteoform discovery and identification: Addressing sample complexity in top-down**

native ambient mass spectrometry; Oliver Hale¹; Rosa Viner²; Weijing Liu²; Rafael Melani²; Christopher Mullen²; Helen Cooper¹; ¹University of Birmingham, Birmingham, United Kingdom; ²Thermo Fisher Scientific, San Jose, CA

TOG am 09:10 **Native Top-Down MS with a Tribrid Orbitrap System Reveals Higher Order Structure Information for Protein Complexes;** Bovu Zhao¹; Jessie Le¹; Christopher Mullen²; Jingjing Huang²; Rafael Melani²; Joseph Loo¹; ¹UCLA, Los Angeles, CA; ²Thermo Fisher Scientific, San Jose, CA

TOG am 09:30 **Hybrid mass spectrometric approaches on Orbitrap and timsTOF platforms aimed at deciphering human antibody repertoires;** Albert J.R. Heck; ¹Utrecht University, Utrecht, Netherlands

TOG am 09:50 **Global Proteoform Analysis in Human Hypertrophic Cardiomyopathy through Top-Down Proteomics;** Zhan Gao¹; Kalina J Rossler¹; Holden T Rogers¹; Timothy J Aballo¹; Emily A Chapman¹; Matthew S Fischer¹; Boris Krichel¹; Yanlong Zhu¹; Ying Ge¹; ¹UW-MADISON, Madison, WI

TOG am 10:10 **New bioinformatics tools for de novo sequencing of complex protein spectra;** Mariangela Kosmopoulou¹; George Alevizos¹; Georgia Orfanoudaki¹; Athanasios Smyrnakis¹; Stuart Pengelley²; Detlev Suckau²; Dimitris Papanastasiou¹; ¹Fasmatech, Athens, Greece; ²Bruker Daltonics GmbH & Co.KG, Bremen, Germany

TOH am: Informatics: Metabolomics and Lipidomics Room 303ABCD (Level 3)

Session Chair: Xiaoyu Sara Yang (National Institute of Standards & Technology (NIST))

TOH am 08:30 **Standardizing nontargeted metabolomics and exposomics: The LC-BinBase environment;** Oliver Fiehn¹; Yuanyue Li¹; Huaxu Yu¹; Parker Bremer¹; Fanzhou Kong¹; Diego Pedrosa¹; Daniel Rundle¹; Uri Keshet¹; Tong Shen¹; Gert Wohlgemuth¹; ¹UC Davis, Davis, CA

TOH am 08:50 **MS-DIAL 5 multimodal mass spectrometry data mining unveils lipidome complexities;** Hiroshi Tsugawa¹; Hiroaki Takeda²; Yuki Matsuzawa³; Manami Takeuchi³; Mikiko Takahashi⁴; Kozo Nishida³; Takeshi Harayama⁵; Yoshimasa Todoroki³; Kuniyoshi Shimidzu³; Nami Sakamoto³; Takaki Oka³; Masashi Maekawa³; Mi Hwa Chung³; Yuto Kurizaki³; Saki Kiuchi³; Kanako Tokiyoshi³; Bujinlkham Buyantogtokh³; Misaki Kurata³; Aleš Kvasnička⁶; Ushio Takeda⁷; Haruki Uchino⁸; Mayu Hasegawa⁹; Junki Miyamoto⁹; Kana Tanabe¹⁰; Shigenori Takeda¹⁰; Tetsuya Mori¹¹; Ryota Kumakubo³; Tsuyoshi Tanaka³; Tomoko Yoshino³; Makoto Arita¹²; ¹Tokyo University of Agriculture and Technology, Tokyo, Japan; ²Tokyo University of Agriculture and Technology, Koganei-shi, Japan; ³Tokyo University of Agriculture and Technology, Koganei-shi, Japan; ⁴RIKEN Center for Sustainable Resource Science, Yokohama, Japan; ⁵CNRS UMR7275, 660 Route des Lucioles, France; ⁶University Hospital Olomouc, Zdravotníku, Czech Republic; ⁷K.K. ABSciex, Shinagawa, Japan; ⁸RIKEN Center for Integrative Medical Sciences, Yokohama, Japan; ⁹Tokyo University of Agriculture and Technology, Fuchu, Japan; ¹⁰AGC, Yokohama, Japan; ¹¹RIKEN CSRS, Yokohama, Japan; ¹²Graduate School of Pharmaceutical Sciences, Keio University, Minato-ku, Japan

TOH am 09:10 **Approximately Perfect: How to retrieve meaningful molecular structure hits from MS/MS data for small molecule annotation;** Martin A. Hoffmann¹; Marcus Ludwig¹; Kai Dührkopf²; Markus Fleischauer²; Nils A. Haupt²; Fleming Kretschmer²;

TUESDAY ORALS

- Sebastian Böcker²; ¹Bright Giant GmbH, Jena, Germany; ²Friedrich Schiller University Jena, Jena, Germany
- TOH am 09:30 **LipStR - Statistical analyses and Visualization of quantitative mass spectrometry-based lipidomic experiments**; Anatoly Belov¹; William Dishen Liu¹; Weng Ruh Wong¹; James Joubert¹; Qingling Li¹; Wendy Sandoval¹; Meena Choi¹; ¹Genentech, Inc., South San Francisco, CA
- TOH am 09:50 **The ALEX score: a universal metric for confident lipid identification**; Jürgen Hartler^{1, 2}; Leonida M. Lamp¹; Christer S. Ejsing^{3, 4}; ¹Pharmaceutical Sciences, University of Graz, Graz, Austria; ²Field of Excellence BioHealth, University of Graz, Graz, Austria; ³Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense, Denmark; ⁴Cell Biology and Biophysics Unit, European Molecular Biology Laboratory (EMBL), Heidelberg, Germany
- TOH am 10:10 **Using ADAP-BIG to curate a benchmarking dataset generated for evaluating software tools for preprocessing mass spectrometry-based metabolomics data**; Xiuxia Du¹; Linxing Yao²; Nathan Montgomery²; Kevin Cho³; Gary Patti³; Corey Broeckling²; ¹University of North Carolina at Charlotte, Charlotte, NC; ²Colorado State University, Fort Collins, CO; ³Washington University in St. Louis, St. Louis, MO
- TOA pm: Cancer Research
Room 210ABC (Level 2)**
Session Chair: Tujin Shi (Pacific Northwest National Laboratory)
- TOA pm 02:30 **The Landscape of Breast Cancer Interactome Aberrations**; Johannes Kreuzer¹; Robert T Morris^{1, 2}; Xcanda I Herrera Lopez^{1, 3}; Soroush Hajizadeh^{1, 4, 5, 6}; Ridwan Ahmad^{1, 5}; Eric F Zaniewski^{1, 5}; Yin Xunquin^{1, 5}; Michael S. Lawrence^{1, 4, 5}; Cyril H Benes^{1, 5}; Dennis C Sgroi^{1, 2, 7}; Wilhelm Haas^{1, 2}; ¹MGH Cancer Center, Charlestown, MA; ²Harvard Medical School, Boston, MA; ³Harvard Medical School, Boston, Massachusetts; ⁴Broad Institute of MIT and Harvard, Boston, MA; ⁵Harvard Medical School, Boston, USA, Massachusetts; ⁶University of Graz, Graz, Austria; ⁷Massachusetts General Hospital, Department of Pathology, Massachusetts General Hospital Cancer Center and Department of Pathology, Harvard Medical School, Boston, USA, Massachusetts
- TOA pm 02:50 **Pan-cancer N-glycoproteomic atlas of patient-derived xenografts for therapeutic target discovery**; Meinusha Govindarajan^{1, 2}; Shahbaz Khan²; Vladimir Ignatchenko²; Nhu-An Pham²; Amanda Khoo^{1, 2}; Lydia Y Liu^{1, 2}; Nazanin Tatar³; Chitra Venugopal³; Laurie Ailles^{1, 2}; Ming-Sound Tsao^{1, 2}; Sheila Singh³; Thomas Kislinger^{1, 2}; ¹Department of Medical Biophysics, University of Toronto, Toronto, ON; ²Princess Margaret Cancer Centre, University Health Network, Toronto, ON; ³Centre for Discovery in Cancer Research, McMaster University, Hamilton, ON
- TOA pm 03:10 **Decrypting the mechanism of action of K-Ras Inhibiting Drugs**; Nicole Kabella¹; Florian P Bayer¹; Amirhossein Sakhteman¹; Johannes Krumm²; Bernhard Kuster¹; ¹Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; ²OmicScouts GmbH, Freising, Germany
- TOA pm 03:30 **Integrated, multidimensional, proteomic and metabolomic characterization of oligodendrogloma to uncover foundational rare brain tumor biology**; Bianca Janine Kuhn¹; Natalie M Clark¹; C Williams¹; Jackson White¹; Joe D Allen¹; Karl Clauser¹; Mateusz P Kopytra²; Yuankun Zhu²; Zhang Bo²; Adam C Resnick²; Dhiraj Dokwal^{3, 4}; Brock Greene⁵; Steven A. Carr¹; DR Mani¹; Samuel McBrayer⁴; Shankha Satpathy¹; Michael A. Gillette¹; ¹Broad Institute of MIT and Harvard, Cambridge, MA; ²Children's hospital of Philadelphia, Philadelphia, Pennsylvania; ³UT Health Science Center at San Antonio, San Antonio, TX; ⁴University of Texas Southwestern Medical Center, Dallas, TX; ⁵Oligo Nation, Sebastopol, CA
- TOA pm 03:50 **Proteogenomic Characterization of High-Grade Endometrial Cancers**; Nicholas W. Bateman¹; Tamara Abulez¹; Sakiyah Taqee¹; Julie Oliver¹; Kelly A Conrads¹; Brian L Hood¹; Douglas Craig²; Gregory Dyson²; Julie Boerner²; Neil T Phippen¹; Christopher M Tarney¹; Kathleen M Darcy¹; Mohamed Elshaikh²; Rouba Ali-Fehmi²; Michele Cote²; George L Maxwell¹; Thomas P Conrads¹; ¹Women's Health Integrated Research Center, Annandale, VA; ²Wayne State University, Detroit, MI
- TOA pm 04:10 **Spatial multi-omics investigation of high-grade serous ovarian cancer tumor microenvironment provides insight into minimal residual disease and intrinsic chemoresistance**; Erin Seeley¹; Basant Gamal²; Akshay Bas³; Nathan Heath Patterson⁴; Wanqiu Zhang⁴; Maria José Q Mantas⁴; Alice Ly⁴; Nico Verbeek⁴; Marc Claesen⁴; Amir Jazaeri²; Jared Burks³; Samuel Mok²; Sammy Ferri-Borgogno²; ¹Department of Chemistry, University of Texas at Austin, Austin, TX; ²Department of Gynecologic Oncology and Reproductive Medicine, The University of Texas MD Anderson Cancer Center, Houston, TX; ³Department of Leukemia, The University of Texas MD Anderson Cancer Center, Houston, TX; ⁴Aspect Analytics, Genk, Belgium
- TOB pm: Ion Mobility: Structure Determination & Applications
Room 207ABC (Level 2)**
Session Chair: Brandon Ruotolo (University of Michigan)
- TOB pm 02:30 **Characterizing a Surface Salt Bridge in the Four-Helix Bundle Rop by Surface-Induced Activation and Variable Temperature Electrospray Ionization**; Kristie L Baker¹; Anusha Kumar¹; Aniruddha Sahasrabudde¹; Hossein Ashrafian¹; Thomas J. Magliery¹; Vicki H. Wysocki¹; ¹The Ohio State University, Columbus, OH
- TOB pm 02:50 **An IMS-MS Method for Characterization of Diastereomer Content in PS-Modified Synthetic Oligonucleotides**; Edith Sharon¹; Sarah O'Keefe¹; Shannon Raab²; Kathleen Grassmyer²; Todd Maloney²; David Clemmer¹; ¹Indiana University, Bloomington, IN; ²Eli Lilly & Company, Indianapolis, IN
- TOB pm 03:10 **Efforts Towards True High Throughput Native MS to Elucidate Structural Characterization of Biopharmaceutical Proteins using Ion-Mobility and Collision Induced Unfolding**; Kristine F Parson¹; Margo Wilson¹; Mason Chilmonecny²; Austin Culberson²; Jason Barker¹; Adam Conner¹; Greg Adams¹; ¹FUJIFILM Diosynth Biotechnologies USA, Inc, Morrisville, North Carolina; ²Andson Biotech, Atlanta, GA
- TOB pm 03:30 **Development of a MALDI-IMS-MS Tool for Amino Acid Stereochemistry Analysis**; Jiaxuan Yan¹; Xing Yin¹; Hillary A Schuessler¹; Douglas D Richardson¹; Wendy Zhong¹; ¹Merck & Co., Rahway, NJ
- TOB pm 03:50 **The Effects of Experimental Conditions and Instrument Settings on Mass Spectral Library Identifications while Using Ion Mobility**; Yamil Simón-Manso¹; Meghan C Burke¹; Brian T. Cooper^{1, 2}; Tytus Mak¹; Yuxue Liang¹; William E. Wallace¹; Stephen E Stein¹; ¹NIST, Gaithersburg, MD; ²Department of Chemistry, University of North Carolina, Charlotte, North Carolina
- TOB pm 04:10 **An Interlaboratory Evaluation of Collision Cross Section Measurements from a Plasma Lipid**

TUESDAY ORALS

Extract on a Commercial SLIM Ion Mobility Platform; Rachel Harris¹; Emanuel Zlibut¹; Sarah M. Stow²; Allison R Reardon³; Kyle E Lira³; David L Williamson⁴; Jody C May³; Michelle English¹; Jennifer Krone¹; Komal Kedia⁵; John A McLean³; Frederick G. Strathmann¹; ¹MOBILion Systems, Inc., Chadds Ford, PA; ²Agilent Technologies, Santa Clara, CA; ³Vanderbilt University, Nashville, TN; ⁴University of Utah, Salt Lake City, UT; ⁵Merck & Co., Inc., West Point, PA

TOC pm: Fundamentals: Ion Structures, Energetics, and Reactions (Honoring Jack Beauchamp) Room 304AB (Level 3)

Session Chair: Peter Armentrout (University of Utah)

- TOC pm 02:30 **Celebrating Jack Beauchamp's Career upon the Advent of his Retirement;** Nathan Dalleska; Caltech, Pasadena, CA
- TOC pm 02:50 **Influence of Modifications on the Base Pairing of Protonated Cytidine Hetero-Nucleoside Base Pairs: Implications for i-Motif Assembly and Stability;** Mary T Rodgers; Wayne State University, Detroit, MI
- TOC pm 03:10 **Time-resolved Collision-induced Unfolding of Small Molecules Probed Using CRAFTI Techniques;** Noah J Mismash¹; Kelley Kim¹; David V Dearden¹; ¹Brigham Young University, Provo, UT
- TOC pm 03:30 **Investigation of Uranyl Perchlorate Anion Complexes in the Gas Phase via Infrared Multiphoton Dissociation and Collision Induced Dissociation;** Brittany DM Hodges¹; Christopher A. Zarzana¹; JungSoo Kim¹; Jonathan K. Martens²; Giel W.C.M. Berden²; Jos Oomens²; ¹Idaho National Laboratory, Idaho Falls, ID; ²FELIX Laboratory - Radboud University, Nijmegen, Netherlands
- TOC pm 03:50 **Site-specific photodissociation of peptide bonds: a new tool for top-down proteomics;** Ryan R. Julian; University of California, Riverside, Riverside, CA
- TOC pm 04:10 **Amyloid Disease Oligomer Assembly Mechanisms: ALS and Parkinson's Disease Core Peptides Form Long Lived Toxic Cylindrins and Beta Barrels;** Michael T. Bowers¹; Yingying Jin¹; Zhiyuan Zhu¹; Steven Buratto¹; ¹University of California, Santa Barbara, CA

TOD pm: Food Safety & Chemistry: Innovations Room 304CD (Level 3)

Session Chair: Karen E. Butler (FDA, Joint Institute for Food Safety and Applied Nutrition)

- TOD pm 02:30 **A robust and sensitive parallel reaction monitoring mass spectrometry method for quantifying egg proteins from multiple processed food matrices;** Liyun Zhang¹; Philip Johnson¹; Melanie Downs¹; ¹Food Allergy Research and Resource Program, Department of Food Science and Technology, University of Nebraska-Lincoln, Lincoln, Nebraska, Lincoln, NE
- TOD pm 02:50 **Determining C=C Bond Positions in Unsaturated Fatty Acids and Phospholipid Fatty Acyl Chains Using Rapid Evaporative Ionization Mass Spectrometry (REIMS);** Thomas G Milnes¹; Nicholas Birse²; Simon JS Cameron²; ¹Queens University Belfast, Belfast, United Kingdom; ²Queens University Belfast, Belfast, United Kingdom
- TOD pm 03:10 **The End-to-end Workflow for Analysis of Per- and Polyfluoroalkyl Substances (PFAS) in Infant and Baby Young Children Food;** Limian Zhao¹; Matthew Giardina¹; Emily Parry¹; ¹Agilent Technologies, Wilmington, DE
- TOD pm 03:30 **Nontargeted and suspect screening of per- and polyfluoroalkyl substances (PFAS) in food contact materials;** Craig Butt¹; Holly Lee²; ¹SCIEX, Framingham, MA; ²SCIEX, Concord, ON

TOD pm 03:50 **A Limited Sample Deep Learning Model for LC-MS to Authenticate Consumer Products;** Pulasthi Ekanayake¹; Osanda Hemachandra¹; Andi Krupke¹; Lalin Theverapperuma¹; Doreen Chrisanthy¹; ¹Expert Intelligence, Santa Clara, CA

TOD pm 04:10 **Food for Thought: Characterizing 500 Commonly Consumed Foods through Standardized Metabolomics for The Periodic Table of Food Initiative;** Arpana Vaniya¹; Jessica E. Prenni²; Jacqueline Michelle Chaparro²; Melanie Odenkirk²; Margaret Read²; Susan B. Mitchell²; Corey D. Broeckling²; Nathan Montgomery²; Nichole Reisdorph³; Richard Reisdorph³; Cole Michel³; Katrina A. Doenges³; Oliver Fiehn¹; Stacy D. Sherrod⁴; Katrina L. Leaprot⁴; Jody C. May⁴; John A. McLean⁴; Chi-Ming Chien⁵; Tracy Shafizadeh⁵; Steve Watkins⁵; ¹UC Davis, Davis, CA; ²Colorado State University, Fort Collins, CO; ³University of Colorado, Anschutz Medical Campus, Department of Pharmaceutical Sciences, Aurora, CO; ⁴Vanderbilt University, Nashville, TN; ⁵Verso Biosciences, Davis, CA

TOE pm: Single Cell Omics Ballroom DE (Level 3)

Session Chair: Fabio Gomes (Virginia Commonwealth University)

- TOE pm 02:30 **Capillary Electrophoresis Mass Spectrometry for Deep Single-Cell Proteomics;** Bowen Shen¹; Fei Zhou¹; Peter Nemes¹; ¹University of Maryland, College Park, College park, MD
- TOE pm 02:50 **High-throughput, single-cell top-down proteomics using multisegmented spray-capillary CE-MS;** Zhitao Zhao¹; Yanting Guo¹; Trishika Chowdhury²; Samin Anjum²; Jiaxue Li¹; Lushuang Huang¹; Kellye A. Cupp-Sutton²; Anthony Burgett³; Dingjing Shi¹; Si Wu^{1, 2}; ¹Oklahoma University, Norman, OK; ²University of Alabama, Tuscaloosa, AL; ³Oklahoma Medical Research Foundation, Oklahoma City, Oklahoma
- TOE pm 03:10 **Single-nucleus proteomics identifies regulators of subcellular protein transport in LPS-stimulated macrophages;** Jason Derks¹; Tobias Jonson¹; Andrew Leduc¹; Luke Khoury¹; Saad Khan¹; Nikolai Slavov^{1, 2}; ¹Northeastern University, Boston, MA; ²Parallel Squared Technology Institute, Watertown, MA
- TOE pm 03:30 **Automated single-cell and spatial proteomics workflows to enable in-depth tissue mapping;** Claudia Ctorteka¹; Natalie M Clark¹; Brian Boyle¹; Anjali Seth²; Moe Haines¹; Namrata D. Udeshi¹; Michael A. Gillette^{1, 3}; Shankha Satpathy¹; Steven A. Carr¹; ¹Broad Institute of MIT and Harvard, Boston, MA; ²Cellenion, Lyon, France; ³Massachusetts General Hospital (MGH), Charlestown, MA
- TOE pm 03:50 **Same single-cell co-profiling of proteomes and transcriptomes from human pancreas with spatial resolution;** James M Fulcher¹; Lye Meng Markillie²; Hugh D Mitchell²; Sarah M Williams²; David J Degnan³; Lisa M Bramer³; Liang Chen²; Rashmi Kumar²; Joshua Cantlon-Bruce⁴; Johannes W Bagnoli⁵; Wei-Jun Qian³; Anjali Seth⁵; Ljiljana Paša-Tolić²; Ying Zhu⁶; ¹Pacific Northwest National Lab, Richland, WA; ²Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA; ³Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; ⁴Sciencion US, Tempe, AZ; ⁵Cellenion, Lyon, France; ⁶Genentech Inc, South San Francisco, CA
- TOE pm 04:10 **Single Cell Analysis of Proteoforms Using single-cell proteoform imaging mass spectrometry (scPiMS);** Pei Su¹; Michael A. Hollas¹; Fatma Ayaloglu Butun¹; Vijaya Lakshmi Kanchustambham¹; Stanislav Rubakhin²; Namrata

TUESDAY ORALS

Ramani¹; Joseph B. Greer¹; Bryan P. Early¹; Ryan T. Fellers¹; Michael A. Caldwell¹; Jonathan V. Sweedler²; Jared O. Kafader¹; Neil L. Kelleher¹; ¹Northwestern University, Evanston, IL; ²University of Illinois at Urbana-Champaign, Urbana, IL

TOF pm: Immunopeptidomics: MS Methods Ballroom C (Level 3)

Session Chair: Aleksandra Nita-Lazar (NIH/NIAID/LISB)

TOF pm 02:30 **DIA for immunopeptidomics: assessment of quantitative accuracy and ability to detect HLA-I peptides from common cancer neoantigens**; Denys Oliinyk¹; Hem Gurung²; Christopher M Rose²; Susan Klaeger²; ¹Universitätsklinikum Jena, Jena, Germany; ²Genentech Inc., South San Francisco, CA

TOF pm 02:50 **MS-based immunopeptidomics to expand the landscape of robust antigens for immunotherapy in chronic lymphocytic leukemia (CLL)**; Maria Virginia Ruiz Cuevas¹; Karl R. Clauser¹; Jennifer G. Abelin¹; Suzanna Rachimi¹; Kshiti Meera Phulphagar¹; Claudia Ctorteca¹; D. R. Mani¹; Marwan Kwok²; Catherine Wu^{1, 2}; Steven A. Carr¹; ¹Broad Institute of MIT and Harvard, Cambridge, MA; ²Dana-Farber Cancer Institute/ Harvard Medical School, Boston, MA

TOF pm 03:10 **Identification of tumor antigens for cancer immunotherapy against non-small cell lung cancer**; Chantal Durette¹; Eric Bonneil¹; Lilian R Heil²; Anca Apavaloaei^{3, 4}; Joel Lanoix³; Marie-Pierre Hardy³; Krystel Vincent³; Tonya Pekar-Hart²; Claude Perreault^{3, 5}; Pierre Thibault^{3, 6}; ¹IRIC Université de Montréal, Montréal, Québec; ²ThermoFisher Scientific, San Jose, CA; ³IRIC | Université de Montréal, Montreal, QC; ⁴Department of molecular biology, Université de Montréal, Montréal, Québec; ⁵Department of Medicine, Université de Montréal, Montréal, Québec; ⁶Department of Chemistry, Université de Montréal, Montréal, Québec

TOF pm 03:30 **Linear epitopes can be detected with Mass Spectrometry in peptide mixture**; Lona Zenedpour¹; Theo Luidert¹; Maarten Titulaer¹; Marco Schreurs²; ¹Erasmus Medical Center, Rotterdam, Netherlands; ²Microvida, Tilburg, Netherlands

TOF pm 03:50 **Fine tuning of DDA-PASEF methods in combination with ML-assisted rescoring significantly boosts immunopeptide coverage**; Aurélie Hirscher¹; Jeewan Babu Rijal¹; Arthur Declercq^{2, 3}; Lennart Martens^{2, 3}; Christine Carapito¹; ¹BioOrganic Mass Spectrometry Laboratory (LSMBO), IPHC UMR 7178, University of Strasbourg, CNRS, ProFI, Strasbourg, France; ²VIB / UGent - Center for Medical Biotechnology (CMB), Gent, Belgium; ³Department of Biomolecular Medicine, Ghent University, Ghent, Belgium

TOF pm 04:10 **Aberrant mRNA as booster of autoimmune stimulation in cancer**; Alexandra Emanuela Burger¹; Anne-Christine Uldry¹; Sophie Braga-Lagache¹; Oliver Mühlemann¹; Manfred Heller¹; ¹University of Bern, Bern, Switzerland

TOG pm: Structural Biology Ballroom AB (Level 3)

Session Chair: Corinne Lutomski (University of Oxford)

TOG pm 02:30 **The sequential priming mechanism of the progesterone receptor is revealed by structural mass spectrometry**; Matthew D. Mann^{1, 2}; Min Wang³; Michael Patrick Suess³; Anna Malovannaya³; Raj Kumar⁴; Dean P. Edwards³; Patrick R. Griffin²; ¹Scripps Research, Jupiter, FL; ²The Wertheim UF Scripps Institute, Jupiter, FL; ³Baylor College of Medicine, Houston, TX; ⁴Touro College of Pharmacy, New York, NY

TOG pm 02:50 **Characterization of Protein Structure and Proteoforms from Human Heart Tissues by**

Native and Denaturing Top-Down Mass Spectrometry; Emily A Chapman¹; David S Roberts¹; Brad H. Li¹; Boris Krichel^{2, 3}; Zhan Gao⁴; Jáán Andrews¹; Hsin-Ju Chan¹; Man-Di Wang¹; Emily A. Reasoner¹; Kevin M Buck¹; Song Jin¹; Ying Ge^{1, 2, 4, 5}; ¹University of Wisconsin-Madison, Department of Chemistry, Madison, WI; ²University of Wisconsin-Madison, Department of Cell and Regenerative Biology, Madison, WI; ³University of Siegen, School of Life Sciences, Siegen, Germany; ⁴University of Wisconsin-Madison, School of Medicine, Madison, Wisconsin; ⁵Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI

TOG pm 03:10 **Integrating native MS analysis into cryo-EM workflows applied to the structural and functional characterization of SARS-CoV-2 replication-transcription assemblies**; Paul Dominic B. Olinares¹; Gabriel Small¹; Brandon Malone¹; Young Joo Choi¹; James Chen¹; Eliza Llewellyn¹; Seth Darst¹; Elizabeth Campbell¹; Brian T. Chait¹; ¹The Rockefeller University, New York, NY

TOG pm 03:30 **Elucidating Structural Mechanism of GPCR-G Protein Coupling Using High-resolution Mass Spectrometry**; Yi-An Chen¹; Yi-Quan Wang^{1, 2}; Cheng-Han Yu¹; Hsin-Yung Yen¹; ¹Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan; ²Institute of Biochemical Sciences, National Taiwan University, Taipei city, Taiwan

TOG pm 03:50 **Light Induced Conformational Changes in Avian Cryptochromes**; Laila M. N. Shah¹; Angela S. Gehrckens¹; Peter J. Hore¹; Justin L. P. Benesch¹; ¹University of Oxford, Oxford, United Kingdom

TOG pm 04:10 **Charge Detection Mass Spectrometry Reveals Serotype-dependent Differences in the Human Papillomavirus Virus-like Particle Assembly**; Shelby M Klein¹; Lohra M Miller¹; Martin F Jarrold¹; ¹Indiana University Bloomington, Bloomington, IN

TOH pm: High Throughput MS Room 303ABCD (Level 3)

Session Chair: Tawnya Flick (Gilead)

TOH pm 02:30 **Droplet microfluidics coupled to Ion mobility-Mass spectrometry for high throughput screening of isomers from biocatalytic reactions**; Laura I Penabad¹; Alison R.H. Narayan²; Brandon T Ruotolo²; Robert T Kennedy²; ¹University of Michigan-Ann Arbor, Ann Arbor, MI; ²University of Michigan Department of Chemistry, Ann Arbor, MI

TOH pm 02:50 **Rapid Synthesis of Drug Analog Library by High-throughput Desorption Electrospray Ionization (DESI) Mass Spectrometry (MS)**; Kai-Hung Huang¹; Nicolás Morato¹; Yunfei Feng¹; Thomas Sams¹; Eric Dziekonski¹; Graham Cooks¹; ¹Purdue University, West Lafayette, IN

TOH pm 03:10 **High-Throughput Multi-Omics for Bacterial Identification and Antibiotic Susceptibility Profiling**; Hannah Hynds¹; Jana M. Carpenter¹; Kingsley Bimpeh¹; Kelly M. Hines¹; ¹University of Georgia, Athens, GA

TOH pm 03:30 **Are You Kidney Me? Building a Knockout-Proteomics Platform to Identify Novel Targets**; Jeffrey A Culver¹; Max H Russo¹; Pierre J Beltran¹; Joshua Chiou¹; Jason D Arroyo¹; Justin D Crane¹; ¹Pfizer, Cambridge, MA

TOH pm 03:50 **Automating Sample Preparation and Data Processing for the High-Throughput Absolute Quantitation of over 100 HMOs**; Aaron D Stacy¹; Kalyn V Amezcua¹; Anita Vinjamuri¹; Carlito B. Lebrilla¹; ¹UC Davis, Davis, CA

TOH pm 04:10 **Data Driven Targeted Analysis (DTA): Combining Real-Time Artificial Intelligence, DIA, and High Multiplexing for Global Ultra-High Throughput Proteomics**; Soroush Hajizadeh^{1, 2, 3, 4}; Eric F.

TUESDAY ORALS

Zaniewski^{2,5}; Johannes Kreuzer^{2,5}; Daniel A. Haber^{2,5}; Licia V Sequist^{2,5}; Michael S. Lawrence^{2,3,5}; Wilhelm Haas^{2,5}; ¹MGH, Boston, MA; ²Harvard Medical School, Boston, MA; ³Broad Institute of MIT and Harvard, Cambridge, MA; ⁴University of Graz, Graz, Austria; ⁵MGH Cancer Center, Charlestown, MA

WEDNESDAY ORALS

WOA am: Imaging: Spatially-Resolved Omics Room 210ABC (Level 2)

Session Chair: Colleen Crouch (University of Tennessee)

- WOA am 08:30 **Spatial multiomics analysis reveals pro-invasive N-glycosylation changes in the human maternal-fetal interface;** Ke Xuan Leow¹; Inna Averbukh¹; Erin Soon¹; Candace Liu¹; Xiaowei Lu¹; Richard R Drake²; Peggi M Angel²; Sean Bendall¹; Michael Angelo¹; ¹Stanford University, Stanford, CA; ²Medical University of South Carolina, Charleston, SC
- WOA am 08:50 **MALDI-ISH Transcriptomic Spatial Imaging of Alzheimer's Disease Mouse Brain Tissue;** Jonathan M Bell¹; Mark J. Lim¹; Gargey B. Yagnik¹; Kenneth J. Rothschild^{1,2}; ¹AmberGen Inc., Billerica, MA; ²Boston University, Department of Physics and Photonics Center, Boston, MA
- WOA am 09:10 **Metabolome informed proteome imaging to map inflammatory lipid signatures in the micron-scale regions of human placenta tissue;** Marija Velickovic¹; Lisa M Bramer¹; Leena Kadam²; Dušan Veličković¹; Kevin J Zemaitis¹; David J Degnan¹; Jennifer E. Kyle¹; Sarah M. Williams¹; Yuqian Gao¹; Kelly Stratton¹; Matthew E Monroe¹; Ronald J Moore¹; Paul D Piehowski¹; Leslie Myatt²; Kristin E. Burnum-Johnson¹; ¹Pacific Northwest National Laboratory (PNNL), Richland, WA; ²Oregon Health and Science University, Portland, OR
- WOA am 09:30 **Spatial multi-omics guided by SVD k-means ++ clustering and statistical estimation of heterogeneity: Towards dry proteomic guided by lipids MALDI MSI;** Laurine Lagache¹; Yanis Zirem¹; Nawale Hajjaji¹; Zoltan Takats¹; Michel Salzet¹; Isabelle Fournier¹; ¹PRISM - Inserm U1192, Villeneuve d'Ascq Cedex France, France
- WOA am 09:50 **Imaging Post-Translational Modifications in the Sclerotic Subchondral Bone Matrix of Human Knee Osteoarthritis;** Charles A Schurman¹; Jonathon J Woo²; Nannan Tao³; Tamara Alliston²; Peggi M Angel⁴; Birgit Schilling¹; ¹Buck Institute for Research on Aging, Novato, CA; ²University of California-San Francisco, San Francisco, CA; ³Bruker Daltonics, Billerica, MA; ⁴Medical University of South Carolina, Charleston, SC
- WOA am 10:10 **Multimodal Immunofluorescence and Nano-DESI Mass Spectrometry Correlative Imaging of Lipids, Metabolites, Peptides and Proteins;** Manxi Yang¹; Mushfeqa Iqfath¹; Emerson HERNLY¹; Julia Laskin¹; ¹Purdue University, West Lafayette, IN

WOB am: Neuroscience and Neurological Disorders Research Room 207ABC (Level 2)

Session Chair: Nathan Hatcher (Merck Research Labs)

- WOB am 08:30 **Visualizing spatiotemporally resolved interaction networks of G-protein coupled receptors;** Benjamin Polacco¹; Braden T. Lobingier²; Emily E. Blythe¹; Matthew K. Howard¹; Prachi Khare¹; Qiongyu Li¹; Angelina Mullarkey³; Yunting Pu³; Willow Coyote-Maestas¹; Joshua Levitz⁴; Nevan Krogan¹; Mark Von Zastrow¹; Ruth Huttenhain⁵; ¹University of California San Francisco, San Francisco, CA; ²Oregon Health and Science University, Portland, OR; ³Stanford School of Medicine, Palo Alto, CA; ⁴Weill Cornell Medicine, New York, NY; ⁵Stanford University, Stanford, CA
- WOB am 08:50 **Lipidomic profiling in ALS human patients and SOD1/FUS mouse models: a gateway to novel insights into ALS pathogenesis;** Adriana Zardini Buzatto^{1,2}; Sruthi Krishnamurthy³; Caley Campkin⁴; Angela Chan⁵; Francesco Roselli³; Liang Li⁴; ¹University of Calgary, Calgary, AB; ²Calgary Metabolomics Research Facility, Calgary, AB; ³Ulm University, Ulm, Germany; ⁴University of Alberta, Edmonton, AB; ⁵The Metabolomics Innovation Centre (TMIC), Edmonton, AB

- WOB am 09:10 **Mapping Proteoforms Associated with Alzheimer's Disease Through Quantitative Shotgun Top-Down Proteomics of 103 Human Patient Samples;** James M Fulcher¹; Ashley N Ives¹; Evan A Martin²; Sarah M Williams¹; Tom L Fillmore¹; Mowei Zhou³; Ronald J Moore¹; Lei Yu^{4,5}; Phillip L De Jager⁶; David A Bennett^{4,5}; Vladislav A Petyuk²; ¹Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA; ²Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; ³Department of Chemistry, Zhejiang University, Hangzhou, China; ⁴Rush Alzheimer's Disease Center, Rush University Medical Center, Chicago, IL; ⁵Department of Neurological Sciences, Rush University Medical Center, Chicago, IL; ⁶Center for Translational and Computational Neuroimmunology, Department of Neurology & Taub Institute for Research on Alzheimer's disease and the Aging Brain, Columbia University Medical Center, New York, NY

- WOB am 09:30 **Spatial lipidomic profiling of Alzheimer's disease mouse and human tissues using desorption electrospray ionisation mass spectrometry imaging (DESI MSI);** Helen Huang¹; Paolo Ingelese²; Jiabin Tang²; Riad Yagoubi²; Stephane Camuzeaux²; Goncalo Correia²; Anna M Barron³; Steve Gentlemen²; Paul Matthews²; Zoltan Takats²; ¹Imperial College London, London, United Kingdom; ²Imperial College London, London, United Kingdom; ³Nanyang Technological University, Singapore, Singapore

- WOB am 09:50 **Thermal proximity coaggregation reveals mitochondrial dysfunction as a factor in Huntington's Disease pathology;** Josiah E Hutton¹; Tavis J Reed¹; Todd M Greco¹; Joshua L Justice²; Jeffrey P Cantle²; Jeffrey B Carroll²; Ileana M Cristea¹; ¹Princeton University, Princeton, NJ; ²Western Washington University, Bellingham, WA

- WOB am 10:10 **Cerebrospinal fluid proteomics in a multiomic Alzheimer's disease study: emerging insights from a 500-person cohort;** Karl A. T. Makepeace¹; Alexander W. Rookyard¹; Jayanta K. Chakrabarty¹; Anu Jain¹; Min Qiao²; Badri N. Vardarajan²; Lipi Das¹; Min Suk Kang²; Emily G. Werth¹; Dolly Reyes-Dumeyer^{2,3}; Marielba Zerlin-Estevés³; Lawrence S. Honig^{2,3,4}; Lewis M. Brown¹; Richard P. Mayeux^{2,3,4}; ¹Department of Biological Sciences, Quantitative Proteomics and Metabolomics Center, Columbia University, New York, NY; ²Taub Institute for Research on Alzheimer's Disease and the Aging Brain, Department of Neurology, Columbia University Medical Center, New York, NY; ³The Gertrude H. Sergievsky Center, Vagelos College of Physicians and Surgeons, Columbia University, New York, NY; ⁴Department of Neurology, Vagelos College of Physicians and Surgeons, Columbia University and the New York Presbyterian Hospital, New York, NY

WOC am: Drug Metabolism and Pharmacokinetics Room 304AB (Level 3)

Session Chair: Lucinda Hittle (Kallyope, Inc.)

- WOC am 08:30 **Increased throughput of combined stability testing and metabolite identification using sample multiplexing for the development of macrocyclic peptide drugs;** Mark T. Cancilla¹; Congliang Sun¹; Bahanu Habulihaz¹; Lisa A. O'Callaghan¹; Daniel S. Spellman¹; Sven Hackbusch²; Sebastien Morin³; ¹Merck & Co., Inc., West Point, PA; ²Thermo Fisher Scientific, San Jose, CA; ³Thermo Fisher Scientific, Mississauga, ON
- WOC am 08:50 **A Streamlined Data Analysis Workflow for ADC Biotransformation Identification from Intact LC-HRMS data;** Kate Liu¹; Yongling Ai²; Hui Yin Tan¹; Jiaqi Yuan¹; John K. Meissen¹; Yue Huang¹; Anton I.

WEDNESDAY ORALS

- WOC am 09:10 Rosenbaum¹; ¹AstraZeneca, South San Francisco, CA; ²New Jersey Institute of Technology, Newark, NJ
Unveiling Drug Metabolites: A New Software Workflow for De-novo Identification; Mark Sartain¹; Lee Bertram¹; James S Pyke¹; Andrew McEachran¹; Julie Horner-Buxton¹; ¹Agilent Technologies, Santa Clara, CA
- WOC am 09:30 **DMPK of Gefitinib & Gefitinib – PROTAC 3 Following Subcutaneous Administration to the Rat Using Micro Sampling and UPLC-MS/MS**; Robert Plumb¹; Andrew Leightner²; Steven K Lai²; Ian D Wilson³; Amy Bartlett⁴; ¹Waters, Milford, MA; ²Waters Corporation, Milford, MA; ³Imperial College London, London, United Kingdom; ⁴Waters Corporation, Wilmslow, United Kingdom
- WOC am 09:50 **Fast and on-site monitoring of immunosuppressants in liver and renal transplant patients**; Jinling Lu¹; Yinkun Liu¹; Wenpeng Zhang¹; Zheng Ouyang¹; ¹Tsinghua University, Beijing, China
- WOC am 10:10 **Microvolume analysis of antimalarial drugs for pediatric pharmacokinetic studies**; Liusheng Huang¹; Francesca Aweeka²; ¹University of California San Francisco, San Francisco, CA; ²University of California-San Francisco, San Francisco, CA
- WOD am: Exposomics, Toxicology, and Health Outcomes
Room 304CD (Level 3)**
 Session Chair: Silvia Balbo (University of Minnesota)
- WOD am 08:30 **Longitudinal Exposomics in a Wellness Cohort Reveals Distinctive and Dynamic Environmental Chemical Mixtures in Blood**; Kalliroi Sdougkou¹; Stefano Papazian^{1,2}; Benilde Bonnefille^{1,2}; Hongyu Xie¹; Fredrik Edfors²; Linn Fagerberg²; Mathias Uhlén²; Göran Bergström³; Leah JM Martin⁴; Jonathan Martin^{1,2}; ¹Stockholm University, Stockholm, Sweden; ²Science for Life Laboratory (SciLifeLab), Stockholm, Sweden; ³University of Gothenburg, Gothenburg, Sweden; ⁴Independent Researcher, Stockholm, Sweden
- WOD am 08:50 **Employing Various Mass Spectrometry Techniques in Microplastic Biomonitoring and Exposure Risk Assessment**; Kuanliang Shao¹; Sarah Timbie¹; Neha Sehgal¹; Martha Braselton¹; Tim Nawrot²; Runyu Zou³; Mariona Bustamante⁴; Martine Vrijheid⁴; Roel Vermeulen³; Douglas Ian Walker¹; ¹Department of Environmental Health, Rollins School of Public Health, Emory University, Atlanta, Georgia; ²Universiteit Hasselt, Hasselt, Belgium; ³Department Population Health Sciences, Utrecht University, Utrecht, Netherlands; ⁴Institute for Global Health (ISGlobal), Barcelona, Spain
- WOD am 09:10 **Semiquantitative tool for the Nontarget Analysis of Emerging Contaminants in Human Matrices**; Reza Aalizadeh^{1,2}; Varvara Nikolopoulou³; Nikiforos Alygizakis³; Nikolaos S. Thomaidis³; Pablo Gago-Ferrero⁴; Ruben Gil Solsona^{3,4}; ¹Department of Environmental Health Sciences, Yale School of Public Health, Yale University, New Haven, CT; ²Laboratory of Analytical Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Athens, Greece; ³Laboratory of Analytical Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Athens, Greece; ⁴Institute of Environmental Assessment and Water Research (IDAEA-CSIC), Carrer Jordi Girona 18-26, Barcelona, 08034, Spain, Barcelona, Spain
- WOD am 09:30 **A Rapid LC-MS/MS Method for Detecting and Quantifying PFAS Exposures in Sister Study Cohort**; Aishwarya Jala¹; Fariba Tayyari¹; Yeunook Bae¹; Cathelin Huang¹; James L. Burke¹; Che-Jung Chang²; Alexandra White²; Dale Sandler²; William E Funk¹; ¹Northwestern University, Feinberg School of Medicine, Chicago, IL; ²National Institutes of Health (NIH), National Institute of Environmental Health Sciences (NIEHS), Research Triangle Park, North Carolina
- WOD am 09:50 **Leveraging Exposomics and Multi-omics to Investigate the Pathobiology of Asthma**; Peng Gao; University of Pittsburgh, Pittsburgh, PA
- WOD am 10:10 **Rapid detection by SIFT-MS of toxic inorganic and organic compounds relevant to worker safety in the shipping industry**; Paul Wilson¹; Sam Edwards¹; Daniel Comeskey¹; Nathan C Hoppens²; ¹Syft Technologies, Christchurch, New Zealand; ²Syft Technologies, Austin, TX
- WOE am: Instrumentation: High-Resolution Mass Spectrometry
(Honoring Alan Marshall)
Ballroom DE (Level 3)**
 Session Chair: Jon Amster (University of Georgia)
- WOE am 08:30 **Scientific Career of Alan Marshall**; Michael L. Gross; Washington University St. Louis, St. Louis, MO
- WOE am 08:50 **Improved Liquid Chromatography, MS/MS Activation, and Spectral Annotation in High Resolution Mass Spectrometry**; Kristina Hakansson¹; Carson W. Szot¹; Steven A. DeFiglia¹; Menatallah M. Youssef^{1,2}; Neven N. Mikawy¹; ¹University of Michigan Department of Chemistry, Ann Arbor, MI; ²Ain Shams University, Department of Pharmaceutical Analytical Chemistry, Cairo, Egypt
- WOE am 09:10 **ADVANCED FTMS APPROACHES EMPOWER SPATIAL OMICS MEASUREMENTS**; William Kew¹; Kevin J Zemaitis¹; James M Fulcher¹; Mowei Zhou^{1,2}; Dušan Veličković¹; Gregory W Vandergriff¹; Gordon A Anderson³; Matthias Biel⁴; Hamish Stewart⁵; Kyle L. Fort⁵; Maria Reinhardt-Szyba⁵; Tobias Wörner⁵; Alexander A Makarov⁵; Lilijana Paša-Tolić¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²Zhejiang University, Hangzhou, China; ³GAA Custom Electronics LLC, Kennewick, WA; ⁴Embion Software, Ottersberg, Germany; ⁵Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- WOE am 09:30 **A Novel Hybrid Quadrupole-Orbitrap-Ion Trap-FT-ICR Mass Spectrometer**; Chad R Weisbrod¹; Jesse D. Canterbury²; John P. Quinn¹; Lissa C. Anderson¹; Greg T Blakney¹; Amy M McKenna¹; Michael W. Senko²; Alan G Marshall^{1,3}; Christopher L. Hendrickson^{1,3}; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²ThermoFisher Scientific, San Jose, CA; ³Florida State University, Tallahassee, FL
- WOE am 09:50 **Exploiting Mass Differences for Automated Calibration and Data Processing of Complex Mixtures by FT-ICR Mass Spectrometry**; Ryan P. Rodgers^{1,2,3}; Martha L Chacon-Patino^{2,4}; Joseph W Frye-Jones^{4,5}; Alan G Marshall^{4,5}; Alvaro J Tello-Rodriguez^{4,6}; Christopher Holder Montenegro^{4,6}; Germain Salvato Vallverdu^{7,8}; Christopher Rieger⁹; Julien Maillard^{8,10}; Pierre Giusti^{8,10}; Caroline Barrère-Mangote^{8,11}; Carlos Afonso^{8,12}; Brice Bouyssiere^{7,8}; Christopher L Hendrickson^{4,8}; ¹Nat'l High Magnetic Field Lab, Tallahassee, FL; ²International Joint Laboratory (iC2MC), Harfleur, France; ³Université de Pau et des Pays de l'Adour, Pau, France; ⁴National High Magnetic Field Laboratory, Tallahassee, Florida; ⁵Florida State University - Department of Chemistry and Biochemistry, Tallahassee, FL; ⁶Florida State University, Tallahassee, FL; ⁷Université de Pau et des Pays de l'Adour, Pau, France; ⁸International Joint Laboratory – iC2MC : Complex Matrices Molecular Characterization, Harfleur, France; ⁹University of Rostock, Rostock, Germany; ¹⁰TotalEnergies, Harfleur, France; ¹¹TOTALENERGIES OT, Harfleur, France;

WEDNESDAY ORALS

- ¹²University of Rouen-Normandy, Mont-Saint-Aignan, France
- WOE am 10:10 **Characterizing Dynamic MDa Ions Using Fourier Transform Charge Detection Mass Spectrometry**; Conner C. Harper¹; Veena Avadhani¹; Emeline Hanozin¹; Zachary M. Miller¹; Matthew S. McPartlan¹; Evan R. Williams¹; ¹University of California, Berkeley, Berkeley, CA
- WOF am: Chemoproteomics**
Ballroom C (Level 3)
Session Chair: Fleur Ferguson (University of California, San Diego)
- WOE am 08:30 **cysDig: covalent drug discovery via TMT-based targeted proteomics without cysteine enrichment**; Kevin Dong¹; Qing Yu¹; Bertrand Wong¹; Ka Yang¹; Yi-Chi Chu¹; Hong Yue²; Sipei Fu¹; Rebecca L. Whitehouse¹; Miljan Kuljanin¹; Eric Fischer²; Ying Lu¹; Steven P. Gygi¹; ¹Harvard Medical School, Boston, MA; ²Dana-Farber Cancer Institute, Boston, MA
- WOE am 08:50 **Decrypting the molecular basis of cellular drug phenotypes by dose-resolved expression proteomics**; Nicola Beate Berner^{1, 2, 3}; Stephan Eckert^{1, 2, 3}; Karl Kramer¹; Annika Schneider¹; Julian Müller¹; Severin Lechner¹; Sarah Brajkovic¹; Amirhossein Sakhteman¹; Christian Graetz¹; Jonas Fackler⁴; Michael Dudek⁴; Michael Pfaffl¹; Percy Knolle⁴; Stephanie Wilhelm¹; Bernhard Kuster^{1, 2}; ¹Technical University of Munich (TUM), Freising, Germany; ²German Cancer Consortium (DKTK), Partner Site Munich, Munich, Germany; ³German Cancer Research Center (DKFZ), Heidelberg, Germany; ⁴Technical University of Munich (TUM), Munich, Germany
- WOE am 09:10 **29-Plex Click-Compatible Isobaric Tags Enable Highly Multiplexed Proteomics**; Nikolas Burton¹; Daniel A Polasky²; Flowreen Shikwana³; Samuel Ofori¹; Tianyang Yan¹; Daniel J Geiszler²; Felipe Da Veiga Leprevost²; Alexey I Nesvizhskii²; Keriann M Backus¹; ¹UCLA, Los Angeles; ²University of Michigan, Ann Arbor, Michigan; ³UCLA, Los Angeles, California
- WOE am 09:30 **Development of a Mass Spectrometry-Compatible Chemical Probe for Protein Citrullination Enrichment**; Rebecca Meelker Gonzalez^{1, 2}; Sophia Laposchan^{1, 2}; Chien-Yun Lee^{1, 2}; ¹School of Life Sciences, Technical University of Munich, Freising, Germany; ²Young Investigator Group: Mass Spectrometry in Systems Neurosciences, CLINSPECT-M consortium, Freising, Germany
- WOE am 09:50 **Developing and optimizing mass spectrometry methods to improve detection of covalently modified peptides in complex lysates**; Lindsay K Pino¹; Carolyn Allen¹; Daniele Canzani¹; William E Fondrie¹; Yang Gao¹; Tonibelle Gatlinton-Schwager¹; Andrea I Gutierrez¹; Bodhi Hueffmeier¹; Brian McEllin¹; Sebastian Paez¹; Julia Robbins¹; Kyle T Siebenthal¹; Alexander J Federation¹; ¹Talus Bioscience, Seattle, WA
- WOE am 10:10 **Development of a Comprehensive Chemical Proteomics Platform isoBOP-ABPP for High-throughput Quantitative Analysis of Diverse Post-Translational Modifications**; Min Ma¹; Miyang Li²; Hung-Yu Chiang³; Fabao Liu⁴; Xudong Shi⁵; Wei Xu⁴; Kate S Carroll⁶; Lingjun Li^{1, 2}; ¹School of Pharmacy, University of Wisconsin-Madison, Madison, WI; ²Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ³Biophysics Program, University of Wisconsin-Madison, Madison, Wisconsin; ⁴McArdle Laboratory for Cancer Research, University of Wisconsin-Madison, Madison, Wisconsin; ⁵Division of Otolaryngology, Department of Surgery, University of Wisconsin-
- Madison, Madison, Wisconsin; ⁶Department of Chemistry, UF Scripps Biomedical Research, Jupiter, FL
- WOG am: Informatics: Peptide and Protein Identification and Quantification**
Ballroom AB (Level 3)
Session Chair: Brendan MacLean (University of Washington)
- WOG am 08:30 **Improving Quantification in DIA: Insights from the Largest Reported Systematic Study of Ground Truth Experiments**; Monika Pepelnjak¹; Ino Karemaker¹; Christopher Below¹; An-phi Nguyen¹; Oliver M. Bernhardt¹; Sebastian Mueller¹; Roland Bruderer¹; Tejas Gandhi¹; Lukas Reiter¹; ¹Biognosys AG, Schlieren, Switzerland
- WOG am 08:50 **Fixing Percolator: Semi-supervised learning while controlling the false discovery rate**; Jack Freestone¹; Lukas Kall²; William Noble³; Uri Keich¹; ¹University of Sydney, Sydney, Australia; ²Science for Life Laboratory (SciLifeLab), Stockholm, Sweden; ³University of Washington, Seattle, WA
- WOG am 09:10 **Application of the ETHcD method as the only tool for de novo top-down sequencing of intact natural amphibian peptides**; Albert T LEBEDOV¹; Moscow State University, Moscow, Russian Federation; MSU-BIT University, Shenzhen, China
- WOG am 09:30 **Benchmarking Peptide Spectral Library Search**; Hao Xu^{1, 2}; Nuno Bandeira^{1, 2, 3}; ¹Center for Computational Mass Spectrometry, University of California San Diego, La Jolla, CA; ²Department of Computer Science and Engineering, University of California San Diego, La Jolla, CA; ³Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA
- WOG am 09:50 **TEAQ software: automating targeted extraction, evaluation, and assessment of DIA data for the selection of signature peptides for biomarker validation**; Qin Fu¹; Manasa Vegesna¹; Niveda Sundararaman¹; Eugen Damoc²; Tabiwang Arrey²; Anna Pashkova²; Brad Li¹; Jonathan Braun¹; Dermot P.B. McGovern¹; Christopher Murray¹; Yue Xuan²; Jennifer E. Van Eyk¹; ¹Cedars-Sinai Medical Center, Los Angeles, CA; ²Thermo Fisher Scientific, Bremen, Germany
- WOG am 10:10 **The curse of dimensionality in proteomics – a new processing paradigm for DIA data**; Georg Wallmann¹; Patricia Skowronek¹; Marvin Thielert¹; Vincenth Brennstetter¹; Mikhail Lebedev¹; Tim Heymann¹; Constantin Ammar¹; Wen-Feng Zeng¹; Matthias Mann¹; ¹Max Planck Institute of Biochemistry, Planegg, Germany
- WOH am: Fundamentals: Native MS and Structures of Large Ions**
Room 303ABCD (Level 3)
Session Chair: Aneika Leney (University of Birmingham)
- WOH am 08:30 **Fluorinated ethylamines as electrospray-compatible neutral pH buffers for native mass spectrometry**; Brad Davis¹; Algirdas Velyvis¹; Siavash Vahidi¹; ¹University of Guelph, Guelph, ON
- WOH am 08:50 **Real-Time Disulfide Bond Reduction Enabled by Programmed-Temperature Electrospray Ionization (pTESI)**; Theresa A. Gozzo¹; Christopher J. Weir¹; May A. Constabel¹; Meagan M. Gadzuk-Shea²; Matthew F. Bush¹; ¹University of Washington, Seattle, WA; ²AstraZeneca, Waltham, MA
- WOH am 09:10 **Interpreting the conformational dynamics of protein complexes from the thermodynamics measured native mass spectrometry**; He M Sun¹; Thomas Walker^{1, 2}; Morgan Powers¹; Hays Rye¹; Arthur Laganowsky¹; David H Russell¹; ¹Texas A&M University, College Station, TX; ²Agilent Technologies, Wilmington, DE
- WOH am 09:30 **Proteome-specific interactions of highly heterogeneously glycosylated proteins revealed**

WEDNESDAY ORALS

- by super-resolution native mass spectrometry; Tiancheng Lai¹; Yanyi Huang¹; Guanbo Wang¹; ¹Peking University, Beijing, China
- WOH am 09:50 **Orbitrap CD-MS with ultra-long transients exposes distinct ion behavior between empty and filled adeno-associated virus particles; Eduard Ebberink**¹; Victor Yin¹; Evolène Deslignière¹; Arjan Barendregt¹; Tobias P. Wörner²; Anton Kozhinov³; Konstantin Nagornov³; Alisa Ruisinger⁴; Markus Nuebel⁴; Helena Meyer-Berg⁵; Irene R.S. Ferreira⁵; Marco Thomann⁶; Yury O. Tsybin³; Kyle L. Fort²; Alexander A. Makarov²; Albert J.R. Heck¹; ¹Biomolecular Mass Spectrometry and Proteomics, Utrecht University, Utrecht, Netherlands; ²Thermo Fisher Scientific GmbH, Bremen, Germany; ³Spectroswiss, Lausanne, Switzerland; ⁴Roche Diagnostics GmbH, Penzberg, Germany; ⁵Revvity Gene Delivery, Graefelfing, Germany; ⁶Roche Diagnostics GmbH, Penzberg, Germany
- WOH am 10:10 **Native top-down MS of nucleosomes and histone characterization using multiple activation techniques; Nickolas P Fisher**¹; Alexander S Lee^{1,2}; Rafael Melani³; Samuel E Janisse⁴; Matthew R Marunde⁵; Michael-Christopher Keogh⁵; Christopher Mullen⁶; Michael W Senko³; Jared O. Kafader⁴; Neil L Kelleher^{1,4}; ¹Northwestern University, Evanston, IL; ²Northwestern University Feinberg School of Medicine, Chicago, IL; ³Thermo Fisher Scientific, San Jose, CA; ⁴Proteomics Center of Excellence, Northwestern University, Evanston, Illinois; ⁵Epicypther Inc., Durham, NC; ⁶Thermo Fisher Scientific – 355 River Oaks Pkwy, San Jose, California
- WOA pm: Clinical Analysis: Applications**
Room 210ABC (Level 2)
 Session Chair: Mark Molloy (University of Sydney)
- WOA pm 02:30 **Analytical Validation of DESI-MS Imaging for Classification of Thyroid Nodule Biopsies; Rachel J. DeHooq**¹; Monica Lin¹; Ahmed Al-Fartosi¹; Neda Zarrin-Khameh¹; Rongrong Huang¹; James Suliburk¹; Livia S. Eberlin¹; ¹Baylor College of Medicine, Houston, TX
- WOA pm 02:50 **Developing an MRM for typing membranous nephropathy in clinical practice; Aaron J Storey**^{1,2}; Samar Hassen¹; Christian Herzog²; John M Arthur²; Rick D Edmondson²; Tiffany N Caza¹; Chris P Larsen¹; ¹Arkana Laboratories, Little Rock, AR; ²University of Arkansas for Medical Sciences, Little Rock, AR
- WOA pm 03:10 **Investigating rapamycin treatment in older adults with heart failure through metabolomics and lipidomics; Jericha Mill**¹; Isabella James¹; Mandeep Singh²; Judith Simcox^{1,3}; ¹University of Wisconsin-Madison, Department of Biochemistry, Madison, WI; ²Mayo Clinic, Rochester, MN; ³Howard Hughes Medical Institute, Chevy Chase, MD
- WOA pm 03:30 **Multiplexed Quantification of C-Peptide, Proinsulin, and Des-31,32 Proinsulin Proteoforms in Human Plasma by Immunoprecipitation-Nano-LC-MS Assay; Qingqing Shen**¹; Chao Xue¹; Wang Cao¹; Wei-Jun Qian²; Tai-Tu Lin²; Jun Qu^{1,3}; ¹University at Buffalo, buffalo, NY; ²Pacific Northwest National Laboratory, Richland, WA; ³New York State Center of Excellence in Bioinformatics and Life Sciences, buffalo, New York
- WOA pm 03:50 **Investigating Key Host, Variant and Microbial Peptides in Early Oral Carcinogenesis using Advanced Multi-omics Methods; Beverly Wuertz**¹; Ruben Shreshta²; Monica E Kruk³; Subina P Mehta³; Alvaro Sebastian Vaca Jacome²; Matthew Willetts⁴; Frank Ondrey¹; Tim Griffin³; Pratik Dilip Jagtap³; ¹Otolaryngology Department, University of Minnesota, Minneapolis, Minnesota; ²Bruker Scientific LLC, San Jose, CA; ³University of Minnesota, Twin Cities, Minneapolis, MN; ⁴Bruker Scientific, LLC, Billerica, MA
- WOA pm 04:10 **An end-to-end (phospho)proteomics data analysis pipeline for precision oncology of 919 prospective pan-cancer patients; Cecilia Bang Jensen**¹; Amirhossein Sakhteman¹; Annika Schneider¹; Julia Woortman¹; Matthew The¹; Christina Göbel¹; Firas Hamood¹; Moritz Resch¹; Florian P Bayer¹; Christoph Stange¹; Stefan M. Pfister²; Stefan Fröhling²; Chien-Yun Lee¹; Stephanie Wilhelm¹; Bernhard Kuster¹; ¹Technical University of Munich, Freising, Germany; ²DKFZ German Cancer Research Center, Heidelberg, Germany
- WOB pm: H/D Exchange: Innovations and Applications**
Room 207ABC (Level 2)
 Session Chair: Elyssia Gallagher (Baylor University)
- WOB pm 02:30 **Hydrogen-Deuterium Exchange in Traveling Wave Structures for Lossless Ion Manipulations: Advantages and Approaches; Zackary R Kinlein**¹; Haley M Schramm¹; Daniel Wu¹; Brain H Clowers¹; ¹Washington State University, Pullman, WA
- WOB pm 02:50 **Microsecond H/D exchange via an online microfluidic ESI-MS silicon and glass device; Neha Sri Kumar**¹; David Issadore¹; Benjamin A. Garcia²; ¹University of Pennsylvania, Philadelphia, PA; ²Washington University in Saint Louis, St. Louis, MO
- WOB pm 03:10 **Millimeter Water-in-Oil Droplet as an Alternative Back Exchange Prevention Strategy for Hydrogen/Deuterium Exchange Mass Spectrometry of Peptide/Protein; Tin Yi Lui**¹; Tak Wah Dominic Chan¹; ¹The Chinese University of Hong Kong, Hong Kong, Hong Kong
- WOB pm 03:30 **iHX: high sensitivity intensity-based HX-MS2 on an Orbitrap Astral using SRM principles; František Filandr**¹; Vladimir Sarpe¹; David C. Schriemer¹; ¹Department of Biochemistry and Molecular Biology, University of Calgary, Calgary, AB
- WOB pm 03:50 **Quantitative Hydrogen Deuterium Exchange Mass Spectrometry for Rapid Validation and Characterization of Drug Candidates from Small Molecule Libraries; Esther Wolf**¹; Cristina Lento¹; Derek Wilson¹; ¹York University, Toronto, ON
- WOB pm 04:10 **Leveraging HDX-MS to Decipher Protein Stability and Dynamics in Varied Energy Landscapes across Natural and Designed Sequences; Allan J. R. Ferrari**¹; Sugyan Dixit¹; Jane Thibeault¹; Scott Houliston²; Robert Ludwig¹; Mario Garcia¹; Claire Phoumyvong¹; Lauren Carter³; Cheryl H. Arrowsmith²; Miklos Guttman³; Gabriel Rocklin¹; ¹Northwestern University, Chicago, IL; ²University of Toronto, Toronto, ON; ³University of Washington, Seattle, WA
- WOC pm: Fundamentals: Ion Activation and Dissociation**
Room 304AB (Level 3)
 Session Chair: James Prell (University of Oregon)
- WOC pm 02:30 **Spontaneous and Heterogeneous: Ion Emission from ~1 – 40 MDa Aqueous Nanodrops Characterized Using Charge Detection Mass Spectrometry; Matthew S. McPartlan**¹; Conner C. Harper¹; Evan R. Williams¹; ¹University of California, Berkeley, Berkeley, CA
- WOC pm 02:50 **Source-induced Quaternary Structural Changes Revealed by Surface-induced Dissociation and Top-down Electron Capture Dissociation; Andrew J Arslanian**^{1,2}; Vicki H. Wysocki^{1,2}; ¹The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH; ²Native Mass Spectrometry Guided Structural Biology Center, The Ohio State University, Columbus, OH

WEDNESDAY ORALS

- WOC pm 03:10 **Interpreting the Structural Polymorphism of Fc-Fusion Proteins using Ion Mobility-Collision Induced Unfolding (IM-CIU);** Addison E. Bergman¹; Rosendo Villafuerte-Vega¹; Thomas R. Slaney²; Naresh Chennamsetty²; Guodong Chen²; Li Tao²; Devin M. Makey¹; Brandon T. Ruotolo¹; ¹University of Michigan, Ann Arbor, Michigan; ²Bristol Myers Squibb, New Brunswick, NJ
- WOC pm 03:30 **Characterizing the Energy Surfaces of Competing Pathways in Gas-Phase Charge Inversion Ion/Ion Reactions;** Yingchan Guo¹; Jonathan T. Specker¹; Ramón Alain Miranda-Quintana¹; Boone M. Prentice¹; ¹Department of Chemistry, University of Florida, Gainesville, FL
- WOC pm 03:50 **Gas phase investigations on redox-active complexes of the type [M(dgpy)2]n+;** Maximilian Emil Huber¹; Philipp Weber¹; Nathan R. East²; Christoph Riehn¹; Katja Heinze²; Jennifer Meyer¹; ¹RPTU Kaiserslautern-Landau, Kaiserslautern, Germany; ²Johannes Gutenberg University, Mainz, Germany
- WOC pm 04:10 **Orthogonal ion activation modalities implemented on the same instrument for validation of non-canonical lipid isomers;** Samuel C. Brydon¹; Berwyck L.J. Poad¹; Yepy Rustam²; Mengxuan Fang²; Reuben S.E. Young³; Todd W. Mitchell³; Stephen J Blanksby¹; Gavin E. Reid²; David L. Marshall⁴; ¹Queensland University of Technology, Brisbane, Australia; ²University of Melbourne, Melbourne, Australia; ³University of Wollongong, Wollongong, Australia; ⁴Queensland University of Technology, Brisbane, Australia

WOD pm: Environmental: Non-Target Analysis and Emerging Contaminants (In Memory of Ron Hites)
Room 304CD (Level 3)
 Session Chair: John Bowden (University of Florida)

- WOD pm 02:30 **Ronald A Hites: Remembering a "Simple Country Chemist" and his Environmental Analysis Legacy;** Carolyn Koester; Lawrence Livermore National Lab, Livermore, CA
- WOD pm 02:50 **Best Practices for Non-Targeted Analysis (BP4NTA): Developing Tools and Resources to Improve the Usability of NTA Methods and Results;** Christine Fisher¹; Ruth Marfil-Vega²; James McCord³; Sara Nason⁴; ¹FDA, College Park, MD; ²Shimadzu Scientific Instruments, Columbia, MD; ³U.S. Environmental Protection Agency, Research Triangle Park, NC; ⁴The Connecticut Agricultural Experiment Station, New Haven, CT
- WOD pm 03:10 **Predicting solid phase extraction recovery for emerging contaminants and pollutant in wastewater and non-targeted LC/ESI/HRMS analysis;** Amina Souihi¹; Anneli Kruve¹; ¹Stockholm University, Stockholm, Sweden
- WOD pm 03:30 **What's in your wastewater? A nontarget analysis approach to micropollutant identification in residential wastewater treatment systems;** Rachel Smolinski¹; Caitlin Asato²; Meghan Oates²; Stuart Waugh^{2,3}; Christopher J. Gobler^{2,3}; Carrie A. McDonough¹; ¹Carnegie Mellon University, Pittsburgh, PA; ²New York State Center for Clean Water Technology, Stony Brook, NY; ³Stony Brook University, Stony Brook, NY
- WOD pm 03:50 **Deep characterization of PFAS in current and legacy firefighting foam formulations using the Orbitrap Astral mass spectrometer;** Lee Ferguson¹; Marzieh Shojaei¹; Bashar Amer²; Susan S Bird²; ¹Duke University, Durham, NC; ²Thermo Fisher Scientific, San Jose, CA
- WOD pm 04:10 **Targeted and Non-Targeted Analyses of Per- and Polyfluoroalkyl Substances (PFAS) in Dried Blood Spots of Newborns in Southern California;** Sheng Liu¹; Jeremy P. Koelmel^{2,3}; Hazel A.R.

Fajardo²; Katherine Dorazio⁴; Elizabeth Z. Lin²; David Schiessel⁵; Michael Kummer³; David Godri⁶; John Fortner¹; Libby Morimoto⁷; Emma E. Rennie⁸; Veronica Vieira⁹; Catherine Metayer⁷; Krystal J. Godri Pollitt²; ¹Yale University, New Haven, CT; ²Yale School of Public Health, New Haven, CT; ³Innovative Omics, Sarasota, FL; ⁴The Chapin School, New York, NY; ⁵Babcock Laboratories, Inc., Riverside, CA; ⁶3rd Floor Solutions, Toronto, ON; ⁷University of California, Berkeley, Berkeley, CA; ⁸Agilent Technologies, Santa Clara, CA; ⁹University of California, Irvine, Irvine, CA

WOE pm: Instrumentation: New Developments in Ionization and Sampling
Ballroom DE (Level 3)
 Session Chair: Richard Cole (Sorbonne Université)

- WOE pm 02:30 **Developing Technology to Remotely Measure Molecular Composition by Mass Spectrometry;** Sarah Trimpin^{1,2}; Milan Pophristic^{1,3}; Charles N McEwen^{1,3}; ¹MSTM, LLC, Newark, DE; ²Wayne State University, Detroit, MI; ³Saint Joseph's University, Philadelphia, Pennsylvania
- WOE pm 02:50 **Sampling via Sniffing Tube: Direct analysis of large, distant, or otherwise inaccessible samples using ambient mass spectrometry;** Nicole C Auvil¹; Mark E Bier¹; ¹Carnegie Mellon University, Pittsburgh, PA
- WOE pm 03:10 **Direct infusion of on-line liquid-liquid extraction phases for rapid metabolite and lipid profiling;** Ingela Lanekoff¹; Catia Marques¹; Lena Blaase¹; ¹Uppsala University, Uppsala, Sweden
- WOE pm 03:30 **Plasma-Microdroplet Fusion: A Versatile Strategy for Analytical and Preparative Mass Spectrometry;** Abraham Kwame Badu Tawiah¹; Alexander J Grooms¹; Niraj Panday²; Dmytro S Kluyk²; ¹Ohio State University, Columbus, OH; ²Ohio State University, Columbus, OH
- WOE pm 03:50 **High Throughput Single Cell Metabolomic Analysis using Rapid Droplet Sampling Interface Coupled to Mass Spectrometry;** Vilmos Kertes¹; Stephen C Zambrycki¹; John F. Cahill¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN
- WOE pm 04:10 **The nanopore ion source emits amino acid and peptide ions directly into vacuum from a nanoscale aqueous meniscus;** Nicholas Drachman¹; Derek Stein¹; ¹Brown University, Providence, RI

WOF pm: Post-translational Modifications: Qualitative & Quantitative Analysis
Ballroom C (Level 3)
 Session Chair: Hui Zhang (Johns Hopkins University)

- WOF pm 02:30 **Metal ion-decorated ZIC-chILIC StageTip for Simultaneous Profiling of Glycoproteome and Phosphoproteome;** Yi-Ju Chen¹; Yan-Lin Chen¹; Kun-Hao Chang¹; Hsiang-Chun Cheng²; Chiao-Chun Chang²; Yu-Ju Chen^{1,2}; ¹Institute of Chemistry, Academia Sinica, Taipei City, Taiwan; ²Department of Chemistry, National Taiwan University, Taipei, Taiwan
- WOF pm 02:50 **Proteome-wide in vitro kinase and phosphatase assays to determine enzyme-substrate interactions;** Joern Dengjel¹; Melanie Brunner¹; Zehan Hu¹; ¹University of Fribourg, Dept. of Biology, Fribourg, Switzerland
- WOF pm 03:10 **Decrypting lysine deacetylase inhibitor action and protein modifications by dose-resolved proteomics;** Yun-Chien Chang¹; Christian Gnann²; Raphael R. Steimbach^{3,4}; Florian P Bayer¹; Severin Lechner¹; Amirhossein Sakhteman¹; Miriam Abele^{1,5}; Jana Zecha¹; Jakob Trendel¹; Matthew The¹; Emma Lundberg^{2,6}; Aubry K. Miller^{3,7}; Bernhard Kuster^{1,3,8}; ¹Technical University of Munich (TUM), Freising, Germany; ²KTH Royal Institute of Technology,

WEDNESDAY ORALS

- Stockholm, Sweden; ³German Cancer Research Center (DKFZ), Heidelberg, Germany; ⁴Heidelberg University, Heidelberg, Germany; ⁵Bavarian Center for Biomolecular Mass Spectrometry (BayBioMS), Freising, Germany; ⁶Stanford University, Stanford, CA; ⁷German Cancer Consortium (DKTK), Heidelberg, Germany; ⁸German Cancer Consortium (DKTK), Partner Site Munich, Munich, Germany
- WOF pm 03:30 **Probing DNA Damage Signaling and Kinase Specificity with Spatial Resolution;** William Comstock¹; Marcos Navarro¹; Yiseo Rho¹; Marcus B Smolka¹; ¹Cornell University, Ithaca, NY
- WOF pm 03:50 **Exploring PARP1 Auto-modification: Global Insights into DNA Repair during Okazaki Fragment Processing using ETD-based fragmentation;** Jonas Elsborg¹; Sebastian H.N Munk²; Ivo A Hendriks¹; Zita Fábian¹; Michael L Nielsen¹; ¹NNF CENTER FOR PROTEIN RESEARCH, Copenhagen, Denmark; ²Danish Cancer Institute, Copenhagen, Denmark
- WOF pm 04:10 **Exploring the intricate interplay between protein phosphorylation and degradation through highly sensitive sample multiplexing-based quantitative phosphoproteomics with the Orbitrap Astral;** Qing Yu¹; Bertrand Wong¹; Kevin Dong¹; Ka Yang¹; Joao A. Paulo¹; Steven P. Gygi¹; ¹Harvard Medical School, Boston, MA
- WOG pm: Informatics: Multiomics Integration and Applications Ballroom AB (Level 3)**
 Session Chair: Mingxun Wang (University of California, Riverside)
- WOG pm 02:30 **Genetic Modulation of Protein Expression in Rat Brain;** Ling Li¹; Zhiping Wu²; Andrea Guarracino¹; Flavia Villani¹; Deihui Kong¹; Ariana Mancieri²; Aijun Zhang¹; Laura Saba³; Hao Chen¹; Hana Brozka⁴; Karel Vales⁴; Anna N Senko⁵; Gerd Kempermann⁵; Ales Stuchlik⁴; Michal Pravenec⁴; Pjotr Prins¹; Junmin Peng²; Robert W. Williams¹; Xusheng Wang^{1, 2}; ¹University of Tennessee Health Science Center, Memphis, TN; ²St. Jude Children's Research Hospital, Memphis, TN; ³University of Colorado Denver, Aurora, CO; ⁴Institute of Physiology of the Czech Academy of Sciences, Prague, Czech Republic; ⁵Dresden University of Technology, Dresden, Germany
- WOG pm 02:50 **lesSDRF is More: Expanding Proteomics Horizons through Metadata;** Tine Claeys¹; Tim Van Den Bossche¹; Yasset Perez-Riverol²; Kris Gevaert¹; Juan Antonio Vizcaíno²; Lennart Martens¹; ¹VIB - UGent Center for Medical Biotechnology, Gent, Belgium; ²EMBL-EBI, Hinxton, United Kingdom
- WOG pm 03:10 **High-throughput targeted mass spectrometry for detection of novel peptides from bone density-associated protein isoforms predicted by long-read RNA sequencing;** Micah Lehe¹; Erin Jeffery¹; Jennifer Korchak¹; Vasilii Pavelko¹; Charles Farber¹; Gloria Sheynkman¹; ¹University of Virginia, Charlottesville, Virginia
- WOG pm 03:30 **Improve metaproteomics data analysis with a two-pass search workflow in FragPipe;** Yamei Deng¹; Fengchao Yu¹; Alexey I Nesvizhskii¹; ¹University of Michigan, Ann Arbor, Michigan
- WOG pm 03:50 **Comparisons of lipid and RNA spatial distribution in the brains of young and old Alzheimer's and control female murine models;** Amin Jarrahi¹; Lindsay Brown¹; Allison R Jones¹; Alberto F Vargas¹; Kalynn M Schulz¹; Daniel A Jacobson²; Thanh Do¹; Rebecca A Prosser¹; A Colleen Crouch¹; ¹The University of Tennessee Knoxville, Knoxville, TN; ²Oak Ridge National Laboratory, Oak Ridge, TN
- WOG pm 04:10 **Integrated proteomics, lipidomics, and metabolomics reveals molecular landscape perturbations underlying ischemic cardiomyopathy;** Melissa R Pergande¹; Holden T Rogers¹; Kevin M Buck¹; Scott J Price¹; Kalina J Rossler¹; Zhan Gao¹; Timothy J Aballo¹; Paul C Tang²; Ying Ge¹; ¹University of Wisconsin-Madison, Madison, WI; ²Mayo Clinic, Rochester, MN
- WOG pm: Ion Mobility: Instrumentation & Method Development (Honoring Dick Smith) Room 303ABCD (Level 3)**
 Session Chair: Yehia Ibrahim (Pacific Northwest National Laboratory)
- WOG pm 02:30 **Celebrating Dr. Richard D. Smith's Lifelong Efforts Toward Advancing High Performance Mass Spectrometry;** Joseph A. Loo¹; Erin S. Baker²; ¹UCLA, Los Angeles, CA; ²University of North Carolina at Chapel Hill, Chapel Hill, NC
- WOG pm 02:50 **Capturing Arrival Time Distributions Using Phase Shifts, Structures for Lossless Ion Manipulation, and Ion Trap Mass Analyzers (SLIM-Ion Trap MS);** Nathan W. Buzitis¹; Brian H. Clowers¹; ¹Washington State University, Pullman, WA
- WOG pm 03:10 **Hyphenation of ion mobility mass spectrometry and infrared action spectroscopy to probe high order peptide oligomers;** Siors Bakels^{1, 2}; Steve Daly³; Jan Commandeur³; Anouk M. Rijs^{1, 2}; ¹Division of BioAnalytical Chemistry, Vrije Universiteit Amsterdam, Amsterdam, Netherlands; ²Centre for Analytical Sciences Amsterdam, Amsterdam, Netherlands; ³MSVision, Almere, Netherlands
- WOG pm 03:30 **Cyclic ion mobility-mass spectrometry: Towards a direct sequencing of carbohydrates?;** David Ropartz^{1, 2}; Simon Ollivier^{1, 2}; Mathieu Fanuel^{1, 2}; Hélène Rogniaux^{1, 2}; ¹INRAE, UR BIA, Nantes, France; ²INRAE, PROBE Research Infrastructure, BIBS Facility, Nantes, France
- WOG pm 03:50 **Using IM-MS to shape and m/z select ions for microscopy - evaluation of disordered and dynamic proteins;** Hari Newnham¹; Niklas Geue¹; Alexey Barkhanskiy¹; Ellen N Liggett¹; Charles Eldrid¹; Jakub Ujma²; Perdita E Barran¹; ¹The University of Manchester, Manchester, United Kingdom; ²Waters Corporation, Manchester, United Kingdom
- WOG pm 04:10 **Isotopic Ratio and Collision Cross-section Space: An Efficient Approach to Non-targeted Screening of Per-/Polyfluoroalkyl Substances;** Xiaolei Li^{1, 2}; Karl Jobst²; ¹Guangdong Ocean University, Zhanjiang, China; ²Memorial University of Newfoundland, St. John's, NL

THURSDAY ORALS

ThOA am: Biomarkers: Qualitative Analysis Room 210ABC (Level 2)

Session Chair: Yu-Ju Chen (Academia Sinica)

- ThOA am 08:30 **Deep unbiased plasma proteomics biomarker study in a ~3,000 subject multicancer cohort;** Bruce Wilcox¹; Jimmy Yi Zeng¹; Wan-Fang Chou¹; Megan Mora¹; Jacob Waiss¹; Jessica Chan¹; Robert Zawada¹; Jinlyung Choi¹; Sara Nouri Golmaei¹; Joon-Yong Lee¹; Manway Liu¹; Chinmay Belthangady¹; Eltaher Elgierari²; Lee S Cantrell²; Ryan Benz²; Jian Wang²; Serafim Batzoglou²; Philip Ma¹; ¹*PrognomiQ, San Mateo, CA*; ²*Seer, Inc., Redwood City, CA*
- ThOA am 08:50 **Finding classifiers to predict the outcome of neonatal encephalopathy in South African infants;** Annie Moradian¹; Juantia Mellet²; Nathan Hendricks¹; Angel Keseoyan¹; Shruti Rao¹; Jonathan T Bui¹; Monica Ghaly¹; Susan M. Mockus¹; Jeanne Van Rensburg³; Firdose Nakwa⁴; Sithembiso Velaphi⁴; Khomotso Masemola⁵; Shakti Pillay⁶; Alan R Horn⁶; Gugu Kali⁷; Melantha Coetzee⁸; Daynia Ballot⁹; Jennifer E. Van Eyk^{1, 10}; Michael S Pepper²; ¹*Precision Biomarker Laboratories / Cedars-Sinai, Beverly Hills, CA*; ²*Institute for Cellular and Molecular Medicine, Faculty of Health Sciences, University of Pretoria, Pretoria, South Africa*; ³*Institute for Cellular and Molecular Medicine, Faculty of Health Sciences, 2. Institute for Cellular and Molecular Medicine, Faculty of Health Sciences, University of Pretoria, Pretoria, South Africa*; ⁴*Department of Paediatrics and Child Health, Chris Hani Baragwanath Academic Hospital, Faculty of Health Sciences, University of the Witwatersrand, Johannesburg, South Africa*; ⁵*Department of Paediatrics and Child Health, Kalafong Hospital and Faculty of Health Sciences, University of Pretoria, Pretoria, South Africa*; ⁶*Division of Neonatal Medicine, Department of Paediatrics and Child Health, Groote Schuur Hospital, University of Cape Town, Cape Town, South Africa*; ⁷*Department of Paediatrics and Child Health, Stellenbosch University, Tygerberg Hospital Neonatal Unit, Cape Town, South Africa*; ⁸*Department of Paediatrics and Child Health, Division of Neonatology, Steve Biko Academic Hospital, Faculty of Health Sciences, University of Pretoria, Pretoria, South Africa*; ⁹*Department of Paediatrics and Child Health, Charlotte Maxeke Johannesburg Academic Hospital, Faculty of Health Sciences, University of the Witwatersrand, Johannesburg, South Africa*; ¹⁰*Smidth Heart Institute, Cedars-Sinai Medical Center, Los Angeles, CA*
- ThOA am 09:10 **Large parallel reaction monitoring assays for cerebrospinal fluid on a new hybrid nominal mass instrument;** Deanna L. Plubell¹; Philip M. Remes²; Gennifer Merrihew¹; Chris Hsu¹; Nicholas Shulman¹; Brendan MacLean¹; Lilian R Heil²; Jesse D. Canterbury²; Cristina Jacob²; Ping Yip²; William Barshop²; Vane Shen²; Vani Asapu²; Claudia P.B. Martins²; Scott M Peterman²; Michael J. MacCoss¹; ¹*University of Washington, Seattle*; ²*Thermo Fisher Scientific, San Jose, CA*
- ThOA am 09:30 **FAIMS-DIA mass spectrometry-based structural proteomics and N-glycoproteomics in paired cerebrospinal fluid and serum reveals Alzheimer's disease staging biomarkers;** Haiyan Lu¹; Ching-Yuan Yang²; Hua Zhang¹; Zicong Wang¹; Peng-Kai Liu²; Pengshuan Huang³; Lingjun Li^{1, 3}; ¹*School of Pharmacy, University of Wisconsin-Madison, Madison, Wisconsin*; ²*Biophysics Graduate Program, University of Wisconsin-Madison, Madison, Wisconsin*; ³*Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin*
- ThOA am 09:50 **The Human Metabolome Atlas unveils metabolic heterogeneity across cell types and stratifies**

cancer subtypes; Jeremy K Chan¹; William D Gwynne¹; Nicholas S Ly¹; Brandon Y Lieng¹; Olivia Taverniti¹; Mathula Muhundan¹; Alexandra J. Denhart¹; Andrew T Quaille¹; J. Rafael Montenegro-Burke¹; ¹*Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON*

- ThOA am 10:10 **Spatial Mapping of Proteomic Changes Associated with Senescence in Idiopathic Pulmonary Fibrosis;** Rashmi Kumar¹; Yumi Kwon¹; Lorena Rosas²; Liang Chen¹; Kevin J Zemaitis¹; Ana L. Mora²; Mauricio Rojas²; Ljiljana Paša-Tolić¹; ¹*Pacific Northwest National Lab, Richland, WA*; ²*Ohio State University, Columbus, OH*

ThOB am: Fundamentals: Ionization Methods Room 207ABC (Level 2)

Session Chair: Pawel Urban (National Tsing Hua University)

- ThOB am 08:30 **Mapping the optimum spray conditions for oligonucleotides using cVSSI;** Chandrima Banerjee¹; Sultan Mahmud²; Vikum Dewasurendra³; Matthew Johnson³; Stephen J Valentine²; Peng Li²; ¹*West Virginia University, Morgantown, WV*; ²*WVU Department of Chemistry, Morgantown, WV*; ³*WVU Department of Physics, MORGANTOWN, West Virginia*
- ThOB am 08:50 **Advances in Laser- and Lamp-based Photoionization High Resolution Mass Spectrometry: Novel Insights in Complex Mixtures in Energy and Environmental Research;** Christopher Paul Rürger^{1, 2}; Anika Neumann¹; Silvia Vesga-Martínez¹; Fabian Etscheidt^{1, 3}; Ole Tiemann¹; Paul Kösling¹; Carolin Schwarz¹; Lukas Friederici¹; Sven Ehler³; Thorsten Streibel^{1, 4}; Ralf Zimmermann^{1, 4}; ¹*University of Rostock, Institute of Chemistry, Division of Analytical and Technical Chemistry, Rostock, Germany*; ²*International Joint Laboratory – iC2MC : Complex Matrices Molecular Characterization, Harfleur, France*; ³*Photonion GmbH, Schwerin, Germany*; ⁴*Joint Mass Spectrometry Centre, Cooperation Group "Comprehensive Molecular Analytics" (CMA), Helmholtz Munich, Munich, Germany*
- ThOB am 09:10 **Utility of Nanobubbles in Electrospray Ionization Mass Spectrometry: Sensitivity Enhancements and Electrothermal Supercharging Elucidated;** Andre R Venter¹; George Joseph¹; Bincy Binny¹; Roshan Javanshad^{1, 2}; ¹*Western Michigan University, Kalamazoo, MI*; ²*University of Illinois Chicago, Chicago, IL*
- ThOB am 09:30 **Rapid and Sensitive Chemical Analysis of Individual Picoliter Droplets by Mass Spectrometry;** Bryan Bzdek¹; Jim Walker¹; ¹*University of Bristol, Bristol, United Kingdom*
- ThOB am 09:50 **Dynamic Spray Mass Spectrometry;** Purva S. Damale¹; Dmytro S. Kulyk¹; Abraham K. Badu-Tawiah¹; ¹*The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH*
- ThOB am 10:10 **Atomistic Modeling of the ESI Process: From Taylor Cones to Biomolecular Ions and Magic Number Clusters;** Lars Konermann¹; Mahsa Dolatkhan Ouch Bolagh²; Vida Alinezhad²; Kasra Hanifi²; ¹*Univ. of Western Ontario, London, ON*; ²*The University of Western Ontario, London, ON*

ThOC am: Stable Isotope Labeling: Applications Room 304AB (Level 3)

Session Chair: David Goodlett (University of Victoria)

- ThOC am 08:30 **Measuring isotope incorporation in proteins produced using sparse labeling with ¹³C and ¹⁵N;** Elijah T Roberts¹; Hee-Seung Choi¹; Alexander R Davis²; Paul G. Kremer²; Adam W. Barb²; Jon Amster¹; ¹*University of Georgia, Athens, GA*; ²*Department of Biochemistry and Molecular Biology, University of Georgia, Athens, GA*

THURSDAY ORALS

ThOC am 08:50 **Dual 12C/13C curated spectral library of recurrent unidentified LC-HRMS signals obtained from mouse urine labeling to boost human metabolome explorations;** Anais Legrand¹; Sylvain Dechaumet¹; Kathleen Rousseau¹; Laurent Bellanger²; Jean-Jacques Leguay³; Christophe Junot¹; Eric Ezan¹; François Fenaille¹; Annelaure Damont¹; ¹Université Paris-Saclay, CEA, INRAE, Département Médicaments et Technologies pour la Santé (DMTS), MetaboHUB, Gif-sur-Yvette, France; ²Université Paris-Saclay, CEA, INRAE, Département Médicaments et Technologies pour la Santé (DMTS), SPI, Bagnols-sur-Cèze, France; ³UMR 7265 CEA-CNRS-Université Aix Marseille, DRF/Institut de Biosciences et Biotechnologies d'Aix-Marseille (BIAM), plateforme PHYTOTECH, Cité des Energies, Saint-Paul-lez-Durance, France

ThOC am 09:10 **IsoP-SWATH: an unambiguous platform to identify protein modifications;** Rashmi Karki¹; Axe Xie¹; Xingyu Liu¹; Zongtao Lin¹; Francisca N. L. Vitorino¹; Chenfeng Zhao²; Benjamin A Garcia¹; ¹Washington University School of Medicine, St. Louis, MO; ²Washington University in Saint Louis, St. Louis, MO

ThOC am 09:30 **Application of Microdroplet Chemistry for Rapid and Sensitive Measures of Isotope Labeling: Enabling Studies of Glucose Kinetics;** Huifang Yao^{1, 2}; Dan Zhou³; David McLaren¹; Hao Chen²; Stephen Previs¹; ¹Department of Quantitative Biosciences, MRL, Rahway, New Jersey; ²Department of Chemistry & Environmental Science, New Jersey Institute of Technology, Newark, New Jersey; ³Department of In Vivo Pharmacology, MRL, WestPoint, PA

ThOC am 09:50 **Carbon and Nitrogen Positional Isotopomer Determination in Metabolites using Orbitrap IQ-X and a novel hybrid nominal mass instrument;** Rahul Ravi Deshpande¹; Ayush Midha²; Bashar Amer¹; Thomas Moehring³; Isha Jain²; Cristina C. Jacob¹; Susan Bird¹; ¹Thermo Fisher Scientific, San Jose, CA; ²Gladstone Institutes, San Francisco, CA; ³Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

ThOC am 10:10 **Customizable Polymeric Nanocarriers for Interrogating Cellular Metabolism with Hydrophobic Tracers and Drugs;** Michael P Vincent¹; Abigail E Ellis¹; Ryan D Sheldon¹; ¹Van Andel Research Institute, Grand Rapids, MI

ThOD am: Industry: Trace Analysis, Quality Control, and Automation

Room 304CD (Level 3)

Session Chair: Stella Betancourt (Merck Research Labs)

ThOD am 08:30 **Automating Sample Preparation with 3D Printed Hardware for Meso-Scale Proteomics;** Sadie R. Schultz¹; Garrett C. McFadden¹; Matthew M. Champion¹; ¹University of Notre Dame, Notre Dame, IN

ThOD am 08:50 **At-line microchip electrophoresis mass spectrometry analyses to support upstream production of monoclonal antibodies;** Noemí Dorival-García¹; Maikel Gaitkoski¹; Silvia Millán-Martín¹; Josh Smith¹; Sara Carillo¹; Ed Pallister²; Erin Redman²; Milla Neffling²; Morgan Siegmund²; Graziella Piras²; Jonathan Bones^{1, 3}; ¹The National Institute for Bioprocessing Research & Training, Dublin, Ireland; ²908 Devices Inc., Boston, MA; ³School of Chemical and Bioprocess Engineering, University College Dublin, Belfield, Ireland

ThOD am 09:10 **On-line product and process monitoring using photoionization mass spectrometry and hyper fast GC in industrial processes;** Sven Ehlert¹; Andreas Walte¹; Jan Heide^{1, 2}; Kevin Schnepel²; Christian Gehm²; Hendryk Czech^{2, 3}; Ralf

Zimmermann^{2, 3}; ¹Photonion GmbH, Schwerin, Germany; ²University of Rostock, Rostock, Germany; ³Joint Mass Spectrometry Centre, Cooperation Group "Comprehensive Molecular Analytics" (CMA), Helmholtz Munich, Munich, Germany

ThOD am 09:30 **Overcoming the Analytical Challenge of Non-Biological Complex Drug Analysis and Process Control by Combining Comprehensive Chromatographic and Mass Spectrometric Approaches;** Ole Tiemann^{1, 2}; Christopher P. Rüger^{1, 2, 3}; Martha Chacón-Patiño^{3, 4}; Lukas Schwab^{5, 6}; Thomas Gröger⁷; Guido Gayko⁸; Ralf Zimmermann^{1, 2, 6}; ¹Department of Analytical Chemistry, University Rostock, Rostock, Germany; ²Department Life, Light & Matter, University Rostock, Rostock, Germany; ³International Joint Laboratory—iC2MC: Complex Matrices Molecular Characterization, TRTG, BP 27, 76700 Harfleur, France, Harfleur, France; ⁴National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; ⁵University of Rostock, Rostock, Germany; ⁶Joint Mass Spectrometry Centre, Cooperation Group "Comprehensive Molecular Analytics" (CMA), Helmholtz Munich, Munich, Germany; ⁷Helmholtz Munich, Munich, Germany; ⁸Ichthyol-Gesellschaft, Cordes, Hermanni & Co. (GmbH & Co.) KG, Hamburg, Germany

ThOD am 09:50 **Where did all the sulfur go? - A detailed examination of crude oil hydrodesulfurization by FTMS and quantitative LEC-ICP-MS/MS;** Alessandro Vetere¹; Daniel Pröfrock²; Jan T. Andersson³; Wolfgang Schrader¹; ¹Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany; ²Department Inorganic Environmental Chemistry, Institute of Coastal Environmental Chemistry, Helmholtz-Zentrum Hereon, Geesthacht, Germany; ³Institute of Inorganic and Analytical Chemistry, University of Münster, Münster, Germany, Münster, Germany

ThOD am 10:10 **An alternative method to USP <228>, Ethylene Oxide and Dioxane, using the Syft Tracer Pharm11;** K. Chad Bastian¹; Christopher Williams¹; Alyssa McBurney¹; Elliott Franco¹; Leslie P Silva²; Mark J. Perkins³; Vaughan S. Langford⁴; ¹Alcami Corporation, Wilmington, North Carolina; ²Syft Technologies, Los Angeles, CA; ³Element Lab Solutions, Cambridge, United Kingdom; ⁴Syft Technologies, Christchurch, New Zealand

ThOE am: Instrumentation: New Hybrid and Multimodal Approaches

Ballroom DE (Level 3)

Session Chair: Nicholas Riley (University of Washington)

ThOE am 08:30 **Lithium-Ion Battery Electrolyte Compositional Analysis Using Multi-platform mass spectrometry analysis;** Olivier Chevallier¹; Yufeng Zhang²; Aimei Zou³; Jose Meza¹; ¹Agilent Technologies, Santa Clara, CA; ²Agilent Technologies Singapore, Singapore, Singapore; ³Agilent Technologies Singapore, Singapore, Singapore

ThOE am 08:50 **Combinedaldi MSI And AFM Micro-Indentation For Correlation Of Biomechanics And Molecular Composition Of Menisci;** Martina Marchetti-Deschmann^{1, 2}; Aleksandra Lebedeva^{1, 2}; Martin Handelshäuser¹; Lena Hirtler³; Sigfried Trattning³; Benedikt Hager³; Orestis Andreotis¹; Philipp Thurner^{1, 2}; ¹TU Wien, Vienna, Austria; ²ViCEM Vienna Center for Engineering in Medicine, Vienna, Austria; ³Medical University of Vienna, Vienna, Austria

ThOE am 09:10 **An interface between a Cryo-FIB-SEM and Orbitrap Mass Spectrometer;** Aljoscha Körber¹; Hung Q. Hoang²; Olivier De Castro²; Olivier Bouton²;

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- Rachid Barrahma²; Tom Wirtz²; Tobias P. Wörner³; Kyle L. Fort³; Alexander A. Makarov³; Ian G. M. Anthony¹; Ron M. A. Heeren¹; ¹*Maastricht University, Maastricht, Netherlands*; ²*Luxembourg Institute of Science and Technology, Belvaux, Luxembourg*; ³*Thermo Fisher Scientific, Bremen, Germany*
- ThOE am 09:30 **A hybrid online buffer exchange platform for charge-detection mass spectrometry analysis of AAVs and AAV-antibody conjugates**; Chen Du¹; Victoria C. Cotham¹; Shunhai Wang¹; Ning Li¹; ¹*Regeneron Pharmaceuticals, Inc., Tarrytown, NY*
- ThOE am 09:50 **A new adaptation of the Omnitrap platform integrated into a trapped ion mobility time-of-flight mass spectrometer**; Dimitris Papanastasiou¹; Athanasios Smyrnakis¹; Ioannis Orfanopoulos¹; Ilias Panagiotopoulos¹; Rafail Gioves¹; Nikolaos Manolli¹; Mariangela Kosmopoulou¹; Alexandros Lekkas¹; Jean-François Greisch²; Eduardo Carrascosa³; Juergen Suetering³; Stuart Pengelley³; Michael Krause³; Niels Goedecke³; Oliver Raether³; ¹*Fasmatech, Athens, Greece*; ²*Bruker Daltonik GmbH, Fällanden, Switzerland*; ³*Bruker Daltonics GmbH & Co.KG, Bremen, Germany*
- ThOE am 10:10 **Enhancing MS/MS Analysis: A Novel Approach for Improved Multiplexed Mass Spectrometry with Advanced Ion Isolation Techniques**; Linfan Li¹; Philip M. Remes¹; Cristina Jacob¹; ¹*Thermo Fisher Scientific, San Jose, CA*

ThOF am: Lipidomics: New MS Technologies and Applications Ballroom C (Level 3)

Session Chair: Stephen Blanksby (Queensland University of Technology)

- ThOF am 08:30 **Speeding up untargeted lipidomics by 4D-HT-TIMS: Breaking the 5-minute barrier**; Fabrizio Merciai¹; Eduardo Sommella¹; Pietro Campiglia¹; ¹*University of Salerno, Fisciano (SA), Italy*
- ThOF am 08:50 **Lipid profiling with high structural specificity for early detection and progression of cancers**; Xueyun Zheng¹; Dylan H. Ross¹; Richard D. Smith¹; Tao Liu¹; Jennifer E. Kyle¹; ¹*Pacific Northwest National Laboratory, Richland, WA*
- ThOF am 09:10 **Highly sensitive dual-polarity nano-DESI imaging of isomeric lipids in biological tissues**; Sara Amer¹; Daisy M Unishuay Vila¹; Manxi Yang¹; Julia Laskin¹; ¹*Purdue University, Department of Chemistry, West Lafayette, IN*
- ThOF am 09:30 **Advanced high-resolution ion mobility mass spectrometry for enhanced structural glycolipid profiling in human serum**; Huong Giang Vo¹; Sergiu Groppa²; Laura Bindila¹; ¹*Clinical Lipidomics Unit, Institute of Physiological Chemistry, University of Medical Center of the JGU Uni Mainz, Mainz, Germany*; ²*Movement Disorders, Imaging and Neurostimulation, Department of Neurology, University of Medical Center of the JGU Uni Mainz, Mainz, Germany*
- ThOF am 09:50 **Enhancing shotgun ganglioside analysis using class- and charge-based separations by FAIMS**; Katharina Hohenwallner¹; Leonida Lamp²; Madison Nuske³; Liuyu Peng³; Jürgen Hartler²; Gavin E. Reid³; Evelyn Rampler¹; ¹*University of Vienna, Vienna, Austria*; ²*University of Graz, Graz, Austria*; ³*University of Melbourne, Melbourne, Australia*; ⁴*University of Vienna, Vienna, Austria*
- ThOF am 10:10 **Quantification of Enantiomers and Blind Identification of Non-racemates by Cold Ion Spectroscopy**; Oleg V. Boyarkine¹; Vladimir Kopysov¹; Andrei Zviagin¹; Viacheslav Kozlovskii¹; ¹*EPFL, Lausanne, Switzerland*

ThOG am: Artificial Intelligence in MS Instrumentation and Applications Ballroom AB (Level 3)

Session Chair: Magnus Palmblad (Leiden University Medical Center)

- ThOG am 08:30 **MS²DIP: Embracing post-translational modifications for spectrum intensity prediction with molecular embeddings**; Ralf Gabriels^{1, 2}; Alexander Kersert^{1, 2}; Robbin Bouwmeester^{1, 2}; Jasper Zuallaert^{1, 2}; Arthur Declercq^{1, 2}; Alireza Nameni^{1, 2}; Sven Degroev^{1, 2}; Lennart Martens^{1, 2}; ¹*VIB-UGent Center for Medical Biotechnology, Ghent, Belgium*; ²*Department of Biomolecular Medicine, Ghent University, Ghent, Belgium*
- ThOG am 08:50 **A transformer model for de novo peptide sequencing of data-independent acquisition mass spectrometry data**; Justin Sanders¹; Sewoong Oh¹; William S Noble²; ¹*University of Washington, Seattle, WA*; ²*University of Washington - Genome Sciences, Seattle, WA*
- ThOG am 09:10 **DeepQuant: improving data-independent acquisition peptide quantification via unsupervised deep learning-based interference correction**; An-phi Nguyen¹; Monika Pepelnjak¹; Oliver M. Bernhardt¹; Tejas Gandhi¹; Roland Bruderer¹; Lukas Reiter¹; ¹*Biognosys AG, Schlieren, Switzerland*
- ThOG am 09:30 **Real-time prediction of fragmentation and retention time with Salud combined with MSFragger-RTS improves multiplexed immunopeptidome quantification**; Ana Marcu¹; Fengchao Yu²; Susan Klaeger¹; Alexey I. Nesvizhskii²; Christopher M. Rose¹; ¹*Genentech Inc, South San Francisco, CA*; ²*University of Michigan, Ann Arbor, Michigan*
- ThOG am 09:50 **Development of a Continuously Updated Metabolomics Machine Learning Dataset**; Michael Strobel¹; Alberto Gil-de-la-Fuente²; Mohammad Reza Zare Shahneh³; Yasin El Abiead⁴; Mingxun Wang¹; ¹*University of California, Riverside, Riverside, CA*; ²*CEU San Pablo University, Madrid, Madrid*; ³*University of California Riverside, Department of Computer Science, Riverside, CA*; ⁴*University of California, San Diego, La Jolla, CA*
- ThOG am 10:10 **Koina: Bringing machine learning to the community**; Ludwig Lautenbacher¹; Wassim Gabriel¹; Tobias Schmidt²; Marco Schmidt³; Tobias Kockmann³; Christian Panse^{3, 4}; Mathias Wilhelm¹; ¹*Computational Mass Spectrometry, TUM, Freising, Germany*; ²*MSAID, Garching, Germany*; ³*Functional Genomics Center Zurich ETHZ/UZH, Zürich, Switzerland*; ⁴*Swiss Institute of Bioinformatics (SIB), Lausanne, Switzerland*

ThOH am: Biotherapeutics: Characterization and Quantification Room 303ABCD (Level 3)

Session Chair: Weidong Cui (Amgen)

- ThOH am 08:30 **DIA-PTCR resolves spectral congestion on (any?) engineered biotherapeutic**; Wendy Sandoval¹; Christopher Mullen²; Luis Schachner¹; Wilson Phung³; Justin Low³; Benjamin T. Andrews³; Joshua Hinkle²; John E.P. Syka²; Romain Huguet²; Michael T Marty⁴; Rafael Melani²; ¹*Genentech, Inc., South San Francisco, CA*; ²*Thermo Fisher Scientific, San Jose, CA*; ³*Genentech Inc, South San Francisco, CA*; ⁴*University of Arizona, Tucson, AZ*
- ThOH am 08:50 **A Novel Streamlined, Multiplexed In Vitro Expression LC-MS/MS Assay for mRNA Vaccine Development: Method Development to Application**; Leah Wang¹; Olga Friese¹; Kimia Kajbaf¹; Gianna Raymundo¹; Zhenjiu Liu¹; Rachel Edwards¹; Bradley Bare¹; Brian Gau¹; Anji Trujillo¹; Michael Walker¹; Chase Ernsky¹; Emilia Byrne¹; Andrew William Dawdy¹; James Boslett²; Nancy Khoury²; Oleg Jouravlev²; Adam Campbell²; Matthew Thompson³; David Cirelli³; Jason Rouse³; ¹*Pfizer Inc., Chesterfield, MO*; ²*Pfizer Inc., Pearl River, NY*; ³*Pfizer Inc., Andover, MA*

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- ThOH am 09:10 **Advancing Bispecific Antibody Development with Orthogonal Analytical Technologies: A Focus on Cancer Therapeutics**; Andrew D Mahan¹; Kristen Niels²; Zoe Zhang³; Haichuan Liu³; Hirsh Nanda²; ¹Johnson and Johnson, Spring House, PA; ²Johnson and Johnson Innovative Medicine, Spring House, Pennsylvania; ³SCIEX, Redwood City, CA
- ThOH am 09:30 **Characterization of Adeno Associated Virus Therapeutics using Mass Spectrometry Methods**; Shannon Raab¹; Zhirui Lian¹; ¹Eli Lilly and Company, Indianapolis, IN
- ThOH am 09:50 **Best Practices and Tools to Support Consistency of Host Cell Protein Analysis by Mass Spectrometry**; Niomi R Peckham¹; Anthony Blaszczyk¹; Derrick Zhang¹; ¹United States Pharmacopeia, Rockville, MD
- ThOH am 10:10 **ALOX15 is increased during the healing of 2nd degree burn wounds treated with fish skin.**; Ottar Rolfsson¹; Aristotelis Kotronoulas¹; Christian Christiansen¹; Martina Samiotaki²; Hilmar Kjartansson³; Randolph Stone II⁴; ¹University of Iceland, Reykjavik, Iceland; ²Biomedical Sciences Research Center "Alexander Fleming, Athens, Greece; ³Landspítali Háskólasjúkrahús, Reykjavik, Iceland; ⁴US Army Institute of Surgical Research, JBSA Fort Sam Houston, TX
- ThOA pm: Biomarkers: Quantitative Analysis
Room 210ABC (Level 2)**
Session Chair: Annie Moradian (Precision Biomarker Laboratories / Cedars-Sinai)
- ThOA pm 02:30 **A Novel Strategy For The Absolute Quantitation Of Human Proteins**; Vincent R. Richard¹; Robert Popp²; Rene P. Zahedi^{3, 4, 5, 6}; Yassene Mohammed^{1, 7, 8}; Christoph H. Borchers^{1, 8, 9, 10}; ¹Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC; ²MRM Proteomics Inc, Montreal, QC; ³Manitoba Centre for Proteomics and Systems Biology, Winnipeg, MB; ⁴Department of Biochemistry and Medical Genetics, University of Manitoba, Winnipeg, MB; ⁵Department of Internal Medicine, University of Manitoba, Winnipeg, MB; ⁶CancerCare Manitoba Research Institute, Winnipeg, MB; ⁷Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; ⁸Gerald Bronfman Department of Oncology, Jewish General Hospital, Montreal, QC; ⁹Division of Experimental Medicine, McGill University, Montreal, QC; ¹⁰Department of Pathology, McGill University, Montreal, QC
- ThOA pm 02:50 **Automated and generic workflow for ultra-sensitive disease monitoring in multiple myeloma patients using Data Independent Acquisition and an off-the-shelf calibrator**; Charissa Wijnands¹; Gad Armony²; Somayya Noori³; Jolein Gloerich²; Vincent Bonifay⁴; Hélène Caillon⁵; Theo Luiders³; Sven Brehmer⁶; Lennard Pfennig⁶; Gary Kruppa⁷; Tharan Sri Kumar⁸; Thomas Dejoie⁵; Martijn M. Van Duijn³; Alain J. Van Gool²; Joannes F.M. Jacobs¹; Hans Wessels⁹; ¹Laboratory of Medical Immunology, Department of laboratory medicine, Radboud University Medical Center, Nijmegen, Netherlands; ²Translational Metabolic Laboratory, RadboudUMC, Nijmegen, Netherlands; ³Department of Neurology, Erasmus MC, University Medical Center Rotterdam, Rotterdam, Netherlands; ⁴Sebia, Lisses, France; ⁵Biochemistry Laboratory, Hospital of Nantes, Nantes, France; ⁶Bruker Daltonics GmbH & Co.KG, Bremen, Germany; ⁷Bruker S.R.O., Brno, Czech Republic; ⁸Bruker Canada Ltd, Milton, ON; ⁹Translational Metabolic Laboratory, Department of genetics, Radboud University Medical Center, Nijmegen, Netherlands
- ThOA pm 03:10 **Targeted protein analysis of STEAP2 levels across multiple murine FFPE tissues enables the assessment of CAR-T therapy on-target/off-tumor toxicity**; David R. Spicariach¹; Liu Yang¹; Georgina Cornish²; Clare Hoover³; Alexandra Kathenes⁴; Michael Lehmann⁴; Deborah L. Berry⁴; Anton I. Rosenbaum¹; Kévin Contrepois¹; John K. Meissen¹; ¹AstraZeneca, South San Francisco, CA; ²AstraZeneca, Cambridge, United Kingdom; ³AstraZeneca, Waltham, MA; ⁴AstraZeneca, Gaithersburg, MD
- ThOA pm 03:30 **Unraveling potential biomarkers by profiling the crosstalk between miRNA and phosphoproteins in extracellular vesicles from different subtypes of breast cancer**; Jyoti Singh¹; Marco Hadisurya²; Yi-Kai Liu²; Rajesh Singh^{3, 4}; W. Andy Tao^{2, 5, 6}; ¹PURDUE UNIVERSITY, WEST LAFAYETTE, IN; ²Department of Biochemistry, Purdue University, West Lafayette, IN; ³Department of Molecular and Human Genetics, Institute of Science, Banaras Hindu University, Varanasi, India; ⁴Department of Biochemistry, The Maharaja Sayajirao University of Baroda, Vadodara, India; ⁵Department of Chemistry, Purdue University, West Lafayette, IN; ⁶Purdue Institute for Cancer Research, Purdue University, West Lafayette, IN
- ThOA pm 03:50 A Rigorously Controlled, LC-MS-Guided Approach for Obtaining High-Quality Interstitial Fluid from Tissues with Minimal Intracellular Contamination**; Min Ma¹; Shihan Huo¹; Maosheng Wei¹; Shichen Shen¹; Ming Zhang¹; Jun Qu¹; ¹University at Buffalo, Buffalo, NY
- ThOA pm 04:10 **Development of Mass Spectrometry-Based Immunoassay for Microfluidic Paper-Analytical Device for Early Diagnosis of Severe Acute Pancreatitis**; Ruth M Speidel¹; Ella Warner¹; Jona Kozyr-Verni¹; Sophie Miller¹; Georgios Papachristou²; Peter Lee²; Abraham Badu-Tawiah¹; ¹Ohio State University, Columbus, OH; ²Ohio State University Wexner Medical Center, Columbus, OH
- ThOB pm: Plants and Natural Products
Room 207ABC (Level 2)**
Session Chair: Claudia Maier (Oregon State University)
- ThOB pm 02:30 **Bioinformatics-Driven Optimization of Herbal Medicine Development Workflow: Cudrania tricuspidata Leaf Extracts**; Jeong In Seo¹; Hye Hyun Yoo¹; ¹Hanyang University, Ansan, South Korea
- ThOB pm 02:50 **Development of Highly Sensitive and Robust Microflow LC-MS for Comprehensive Metabolomic Profiling of Single Pea Embryo**; Xian Luo¹; Evelyn Osorio²; Alison Ferrie²; HaiYing Yuan²; Liang Li^{1, 3}; ¹The Metabolomics Innovation Centre, Edmonton, AB; ²National Research Council Canada, Saskatoon, SK; ³University of Alberta, Edmonton, AB
- ThOB pm 03:10 **Visualizing fungicide mobility in plant leaves with mass spectrometry imaging**; Akhila Ajith¹; Emrys Jones²; Phillip J Milnes³; Emily Prince³; Giles N Johnson¹; Nicholas P Lockyer¹; ¹University of Manchester, Manchester, United Kingdom; ²Waters Corporation, Manchester, United Kingdom; ³Syngenta, Bracknell, United Kingdom
- ThOB pm 03:30 **Investigation of bacterial-fungal interactions via a simplified model system using mass spectrometry imaging**; Carlismari O. Grundmann¹; Olivia N Matsumoto-Elliott²; Benjamin E Wolfe³; Laura M Sanchez²; ¹University of California Santa Cruz, Santa Cruz, CA; ²University of California, Santa Cruz, Santa Cruz, CA; ³Tufts University, Medford, MA
- ThOB pm 03:50 **RhizoMAP: spatiotemporal metabolic imaging of the rhizosphere**; Dusan Velickovic¹; Tanya Winkler¹; Vimal Balasubramanian¹; Christopher

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Anderton¹; Amir Ahkami¹; Kevin J Zemaitis¹; ¹*PNNL, Richland, WA*
 ThOB pm 04:10 **Unraveling the Molecular Mechanisms of Tomato Fruit Ripening through TMT- and DIA-based Quantitative Proteomics Technologies**; JinJuan Tan¹; Hanqian Feng¹; Zhiping Deng¹; ¹*Institute of Virology and Biotechnology, Zhejiang Academy of Agricultural Sciences, Hangzhou, China*

ThOC pm: GC/MS: Instrumentation and Applications
Room 304AB (Level 3)

Session Chair: Hilkka Kenttämää (Purdue University)

ThOC pm 02:30 **Extending the Range of Compounds and Applications Amenable for Analysis by GC-MS with Cold EI**; Aviv Amirav¹; Benjamin Neumark²; Oleg Elkabets²; Alex Yakovchuk²; Alexander Gordin²; ¹*Tel-Aviv University, Tel-Aviv, Israel*; ²*Tel Aviv University, Tel Aviv, Israel*

ThOC pm 02:50 **Hyphenation of an Dual-Ionization EI&CI-TOFMS with a flow modulated GCxGC system: the ideal combination for compound identification within complex samples**; Steffen Bräkling¹; Sonja Klee¹; Eliska Ceznerova¹; Marleen Vetter¹; Ralf Kurtenbach²; Scott J. Campbell³; John Moncur³; ¹*TOFWERK, Thun, Switzerland*; ²*University of Wuppertal, Wuppertal, Germany*; ³*SpectralWorks Ltd, Runcorn, United Kingdom*

ThOC pm 03:10 **Construction of an in silicoEI mass-spectral library for polymeric material analysis using pyrolysis-GC/MS and machine learning**; Masaaki Ubukata¹; Azusa Kubota¹; Ayumi Kubo¹; John Dane²; ¹*JEOL, Ltd., Tokyo, Japan*; ²*JEOL USA, Inc., Peabody, MA*

ThOC pm 03:30 **FLOW MODULATED GCxGC IN COMBINATION WITH ATMOSPHERIC PRESSURE MASS SPECTROSCOPY USING THE SICRIT IONIZATION SOURCE**; Taylor Hayward¹; Allison Ferranti¹; ¹*Plasmion, Skillman, NJ*

ThOC pm 03:50 **Pyrolysis GC/MS Microplastics Analysis Workflow**; Khadiza Mom; *Quantum Analytics, The Woodlands, TX*

ThOC pm 04:10 **A New Electron Ionization (EI) Source Equipped with a Novel RF Lens Promoting Prolonged Robustness**; Ge Yu¹; Alexander Mordehai¹; Luis Cuadra-Rodriguez¹; Brooke Reaser¹; Elias Feresenbet¹; Nathan Eno¹; Athanasios Nitsopoulos²; Michael Subat²; Raquel Garre-Gallart³; Mari Carmen Saura-Lajarín³; ¹*Agilent Technologies, Santa Clara, CA*; ²*Labor Friedle GmbH, Tegernheim, Germany*; ³*Laboratorio Químico Microbiológico S.L., San Ginés, Spain*

ThOD pm: Challenges in MS Analysis of Complex Mixtures
Room 304CD (Level 3)

Session Chair: Martha Liliana Chacón-Patiño (Florida State University, NHMFL)

ThOD pm 02:30 **Online Liquid Chromatography 21 Tesla FT-ICR Mass Spectrometry Increases Coverage and Confidence of Natural Organic Matter Analysis**; William Kew¹; Rosalie Chu²; Yuri Corilo²; Nicole DiDonato²; Allison Myers-Pigg²; Alan Roebuck²; Kevin J Zemaitis²; ¹*Pacific Northwest National Laboratory, Richland, WA*; ²*Pacific Northwest National Laboratory, Richland, WA*

ThOD pm 02:50 **Comparing Target Screening, Suspect Screening, and Unknown Discovery Workflows in Non-Targeted Analyses of PFAS Using Ion Mobility Mass Spectrometry Data**; Anna K. Boatman¹; Kaylie I. Kirkwood-Donelson²; James N. Dodds¹; Erin S. Baker¹; ¹*University of North Carolina at Chapel Hill, Chapel Hill, NC*; ²*National Institute of Environmental Health Sciences, Durham, NC*

ThOD pm 03:10 **Breaking Through PFAS Characterization Barriers with High-Resolution Ion Mobility**; Mark Strynar¹; Jacqueline Bangma¹; Thomas Lubinsky²;

Jennifer Krone²; Frederick Strathmann²; ¹*US Environmental Protection Agency, Research Triangle Park, NC*; ²*MOBILion Systems, Chadds Ford, PA*

ThOD pm 03:30 **Isomeric Patterns of Benzenesulfonic Acids from Urban Wildfires—"The Mirror Chromatographic Effect" A Tool to Identify Other Isomeric Families**; Michael Thurman¹; Imma Ferrer¹; James S Pyke²; Andrew McEachran²; ¹*University of Colorado, Boulder, CO*; ²*Agilent Technologies Inc., Santa Clara, CA*

ThOD pm 03:50 **Detecting blue-green algae signatures within complex lake samples**; Jaspreet K Sound¹; Aneika C Leney¹; ¹*University of Birmingham, Birmingham, United Kingdom*

ThOD pm 04:10 **Resolving Biology with High Spectral and Spatial Resolution Imaging on a Prototype MALDI TIMS FT-ICR MS**; Madeline E Colley^{1,2}; Martin Dufresne^{1,2}; Alina Theisen³; Lukasz Migas^{1,4}; Cody Marshall^{1,5}; Ali Zahraei^{1,6}; Melissa A. Farrow^{1,6}; Christopher A Wootton³; Raf Van De Plas^{1,4}; Jeffrey M Spraggins^{1,2,5,6,7,8}; ¹*Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN*; ²*Department of Biochemistry, Vanderbilt University, Nashville, TN*; ³*Bruker Daltonik GmbH & Co. KG, Bremen, Germany*; ⁴*Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands*; ⁵*Chemical and Physical Biology Program, Vanderbilt University, Nashville, TN*; ⁶*Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN*; ⁷*Department of Chemistry, Vanderbilt University, Nashville, TN*; ⁸*Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN*

ThOE pm: Instrumentation: Detection of High-Mass Analytes
Ballroom DE (Level 3)

Session Chair: Dalton Snyder (Teledyne FLIR)

ThOE pm 02:30 **Extended m/z range mode of the quadrupole m/z filter on a Tribrid instrument enables precursor m/z selection to 8000 Th**; Christopher Mullen¹; Micahel G. Konicek¹; Graeme C. McAlister¹; Lee Earley¹; Joshua D. Hinkle¹; Rafael Melani¹; John E.P. Syka¹; ¹*Thermo Fisher Scientific, San Jose, CA*

ThOE pm 02:50 **MALDI mass analysis of 26S proteasome and its subunits using MALDI linear ion trap mass spectrometry**; Avinash Adhikrao Patil¹; Ching-Chieh Lee²; Wen-Ping Peng²; ¹*National Dong Hwa University, Shoufeng, Taiwan*; ²*National Dong Hwa University, Shoufeng, Hualien, Taiwan*

ThOE pm 03:10 **High Mass Analysis of Intact mRNAs by Mass Spectrometry and Mass Photometry: The Good, the Bad, and the Ugly**; Evolène Deslignière¹; Lauren F. Barnes²; Thomas Powers²; Olga V. Friese²; Albert J.R. Heck¹; ¹*Biomolecular Mass Spectrometry and Proteomics, Utrecht University, Utrecht, Netherlands*; ²*BioTherapeutics Pharmaceutical Sciences, Pfizer Inc, Chesterfield, MO*

ThOE pm 03:30 **Coupling Online SEC with CD-MS using Hadamard Transform Multiplexing**; James D. Sanders¹; Jeffrey Mosqueira¹; October N Owen¹; Michael T Marty¹; ¹*University of Arizona, Tucson, AZ*

ThOE pm 03:50 **A novel dual sector Charge Detection Mass Spectrometer (CDMS) for Analysis of Adeno-Associated Viruses (AAVs)**; Ellen N Liggett¹; Xudong Wang¹; Alexandros Lekkas²; Yury Tsybin³; Anton N. Kozhinov³; Konstantin Nagornov³; Dimitris Papanastasiou²; Perdita Barran⁴; John B Hoyes^{4,5}; ¹*The University of Manchester, Manchester, United Kingdom*; ²*Fasmatech, Athens, Greece*; ³*Spectroswiss, Lausanne, Switzerland*; ⁴*University of*

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ThOE pm 04:10 *Manchester, Manchester, United Kingdom; ⁵TrueMass, Rowarth, United Kingdom*
Realization of High-Resolution Charge Detection Mass Spectrometry; [David Reitenbach](#)¹; Daniel Y. Botamanenko²; Martin Jarrold³; ¹Indiana University, Bloomington, IN; ²Megadallon Solutions, Bloomington, Indiana; ³Indiana University Bloomington, Bloomington, IN

ThOF pm: Metabolomics: New Technologies and Applications Ballroom C (Level 3)

Session Chair: [Laura-Isobel McCall](#) (San Diego State University)

ThOF pm 02:30 **Digging Deeper into the Unknown: A Low-Mass Optimized High Resolution Ion Mobility Platform for Untargeted Analyses**; Lauren C Royer¹; [Joshua K McBee](#)¹; Leonard Rorrer¹; Miriam Fico¹; Daniel DeBord¹; ¹MOBILion Systems, Inc, Chadds Ford, PA

ThOF pm 02:50 **Metabolomic differentiation of drug MOA in mammalian cell extracts using IR-MALDESI-MS analysis of 350 samples per hour**; [Celeste Sandoval](#)¹; Edward Folk¹; Ary Shalizi¹; Fan Pu²; Nathaniel Elsen²; Phillip Seitzer¹; Jun Xu¹; Zhenghao Chen¹; Andrew Radosevich²; James Sawicki²; Alena Joignant^{2, 3}; Brian Feng¹; Jon Williams²; Bryson Bennett¹; ¹Calico Life Sciences, South San Francisco, CA; ²AbbVie Inc., North Chicago, IL; ³North Carolina State University, Raleigh, NC

ThOF pm 03:10 **Ubiquitous proteomic content and enzymatic activity in metabolomics samples cause post-extraction metabolite changes**; Molly Soper-Hopper¹; Rachel House¹; Michael P Vincent¹; Abigail E Ellis¹; Colt Capan¹; Christine Isaguirre¹; Zachary Madaj¹; Emily Wolfrum¹; Kelsey Williams¹; Hyoungjoo Lee¹; [Ryan D Sheldon](#)¹; ¹Van Andel Institute, Grand Rapids, MI

ThOF pm 03:30 **Simultaneous Quantitation of Multiple Biothiols in Biofluids by Mass Spectrometry using Charged Mass Tags**; [Mousumi Saha](#)¹; Lingqi Qiu¹; Christina R. Ferreira²; Christopher J. Welch³; Yumin Dai⁴; R. Graham Cooks¹; ¹Purdue University, Department of Chemistry, West Lafayette, IN; ²Bindley Bioscience Center, Purdue University, West Lafayette, IN; ³Indiana Consortium for Analytical Sciences & Engineering, Indianapolis, IN; ⁴Takeda Development Corporation, Americas, Cambridge, MA

ThOF pm 03:50 **A valve-based analytical platform with 2D-LC-MS/MS for screening of microperfusion fermentations**; [Sabrina M Cramer](#)^{1, 2}; Shubham Gurav^{1, 2}; David Glinsner^{1, 2}; Sven Kochmann^{1, 2}; Diethard Mattanovich^{1, 2}; Stephan Hann^{1, 2}; Tim Causon^{1, 2}; ¹acib - Austrian Centre for Industrial Biotechnology, Vienna, Austria; ²University of Natural Resources and Life Sciences, Vienna, Austria

ThOF pm 04:10 **Advancing mass spectrometry for systematic characterization of RNA modifications**; Axe Xie¹; [Benjamin A Garcia](#)¹; ¹Washington University School of Medicine, St. Louis, MO

ThOG pm: Quantitative Proteomics: Instrumentation and Applications Ballroom AB (Level 3)

Session Chair: [Thao Nguyen](#) (Calico Life Sciences)

ThOG pm 02:30 **Accelerating relative and absolute quantitative proteomics using broad specificity proteases**; [Xuehui Jiang](#)¹; Darien Yeung^{1, 2}; Yang Liu³; Victor Spicer¹; Havva Afshari^{1, 2}; Louisa Lauenstein¹; Ying Lao¹; Francis Lin³; Oleg Krokhin^{1, 4}; Rene Peiman Zahedi^{1, 2, 4, 5}; ¹Manitoba Centre for Proteomics and Systems Biology, Winnipeg, MB; ²Department of Biochemistry and Medical Genetics, University of Manitoba, Winnipeg, MB; ³Department of Physics and Astronomy, University of Manitoba, Winnipeg, MB; ⁴Department of Internal Medicine, University of

Manitoba, Winnipeg, MB; ⁵Paul Albrechtsen Research Institute, Cancer Care Manitoba, Winnipeg, MB

ThOG pm 02:50 **Deep and economical plasma proteome profiling in a very large cohort to identify biomarkers for adverse pregnancy outcomes**; [Johannes B Müller-Reif](#)¹; Vincent Albrecht¹; Vincenth Brennstetter¹; Medini Steger¹; Waqassuddin Khan^{2, 3}; Aneeta Hotwani⁴; Javairia Khalid^{2, 3}; Imran Nisar^{2, 3}; Fyezah Jehan^{2, 3}; Matthias Mann¹; ¹Max Planck Institute of Biochemistry, Planegg, Germany; ²Department of Pediatrics and Child Health, Faculty of Health Sciences, Medical College, Aga Khan University, Karachi, Pakistan; ³Biorepository and Omics Research Group, Department of Pediatrics and Child Health, Faculty of Health Sciences, Medical College, Aga Khan University, Karachi, Pakistan; ⁴Infectious Diseases Research Lab (IDRL), Department of Pediatrics and Child Health, Faculty of Health Sciences, Medical College, Aga Khan University, Karachi, Pakistan

ThOG pm 03:10 **Instrumentation That Scales Analytical Throughout Reliably And Practically**; [Philip M Remes](#)¹; Cristina C Jacob¹; Oleg Silivra¹; Linfan Li¹; Harald Oser¹; Michael Ugarov¹; Charles Maxey¹; Vane Shen¹; Vani Asapu¹; Yi Liu¹; Jesse D. Canterbury¹; William Barshop¹; Qingyu Song¹; Nicholas Shulman²; Brendan MacLean²; Michael J. MacCoss²; Lilian R Heil¹; Scott M Peterman¹; Neloni Wijeratne¹; Claudia P.B. Martins¹; ¹Thermo Fisher Scientific, San Jose, CA; ²University of Washington - Genome Sciences, Seattle, WA

ThOG pm 03:30 **Quantitative proteome dynamics across embryogenesis in a model chordate**; [Andrea Mariossi](#)¹; Alex Frese¹; Michael Levine¹; Martin Wühr¹; ¹Princeton University, Princeton, NJ

ThOG pm 03:50 **Quantification of Intact Proteins in 100 Human Cells using online high-pH/low-pH nano-RPLC-MS/MS and Tandem Mass Tag Labeling**; [Trishika Chowdhury](#)¹; Kellye A. Cupp-Sutton¹; Yanting Guo²; Anju Teresa Sunny¹; Samin Anjum¹; Zhitao Zhao²; Mai Atallah¹; Si Wu¹; ¹University of Alabama, Tuscaloosa, AL; ²University of Oklahoma, Norman, OK

ThOG pm 04:10 **Leveraging the Orbitrap Astral Mass Spectrometer for TMT and Label-free Data Dependent Acquisition**; Shane L Dawson¹; Yuchen He¹; Qing Yu¹; [Steven P. Gygi](#)¹; Joao A Paulo¹; ¹Harvard Medical School, Boston, MA

ThOH pm: Drug Discovery and Development: Qualitative and Quantitative Analysis Room 303ABCD (Level 3)

Session Chair: [Ashok Dongre](#) (Bristol-Myers Squibb)

ThOH pm 02:30 **Differential ion mobility acoustic ejection MS (DAEMS) system for high-throughput screening of mutase and isomerase enzyme targets**; Patricia Dranchak¹; James Inglese¹; [Tom Covey](#)²; Samad Bazargan²; Chang Liu²; ¹NIH/NCATS, Rockville, Maryland; ²SCIEX, Concord, ON

ThOH pm 02:50 **New-generation automated ambient mass spectrometry platform for high-throughput experimentation in early drug discovery**; [Nicolas M Morato](#)^{1, 2, 3}; Yunfei Feng^{1, 2}; Kai-Hung Huang¹; Beinan Yang⁴; Thomas Sams¹; Kitmin Chen¹; Christina R. Ferreira²; Jiang Yang^{3, 5}; Carleen Klumpp-Thomas⁶; Matt Galbraith⁷; Csaba Hajdu⁸; Steven Pringle⁸; Michael Morris⁸; Julia Balog⁹; Andrew D Mesecar^{3, 4}; R. Graham Cooks^{1, 2, 3}; ¹Department of Chemistry, Purdue University, West Lafayette, IN; ²Bindley Bioscience Center, Purdue University, West Lafayette, IN; ³Purdue Institute for Cancer Research, West Lafayette, IN; ⁴Department of Biochemistry, Purdue University, West Lafayette, IN

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IN; ⁵Department of Comparative Pathobiology, Purdue University, West Lafayette, IN; ⁶National Center for Advancing Translational Sciences, NIH, Rockville, MD; ⁷Hamilton Company, Reno, NV; ⁸Waters Corporation, Wilmslow, United Kingdom; ⁹Waters Corporation, Milford, MA

ThOH pm 03:10 **DrugMap: A quantitative pan-cancer analysis of cysteine ligandability**; Siwen Zhang¹; Mariko Takahashi¹; Harrison Chong¹; Tzu-yi Yang¹; Liron Bar-Peled¹; ¹MGH, Boston, MA

ThOH pm 03:30 **TF-Scan: A high-throughput proteomics platform for transcription factor drug discovery**; Daniele Canzani¹; Julia E Robbins¹; Andrea I Gutierrez¹; J. Sebastian Paez¹; Carolyn Allen¹; Bodhi Hueffmeier¹; Tonibelle Gatbonton-Schwager¹; Yang Gao¹; Kyle T Siebenthal¹; William E Fondrie¹; Alexander J Federation¹; Lindsay K Pino¹; ¹Talus Bioscience, Seattle, WA

ThOH pm 03:50 **Covalent Protein Painting as a novel platform for drug development: identifying off-targets and targets of the Cystic Fibrosis drug Trikafta**; Sandra Pankow¹; Titus H Jung¹; John R. Yates III¹; ¹The Scripps Research Institute, La Jolla, CA

ThOH pm 04:10 **High-throughput and automatable drug target identification using limited proteolysis coupled to mass spectrometry (LiP-MS) suitable for phenotypic screening applications**; Liliana Malinowska¹; Luca Räss¹; Ino Karemaker¹; Vytautas Iesmantavicius²; Fabio Sabino¹; Roland Bruderer¹; Lukas Reiter¹; ¹Biognosys AG, Schlieren, Switzerland; ²Friedrich Miescher Institute for Biomedical Research, Basel, Switzerland