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- MP 002 **Determination of vitamin A, 25-hydroxyvitamin D2/D3 and vitamin E in human serum by UPLC-MS/MS;** Liang Sun<sup>1</sup>; Changkun Li<sup>1</sup>; Yueqi Li<sup>1</sup>; Taohong Huang<sup>2</sup>; <sup>1</sup>Shimadzu (China) Co.,LTD. Beijing Branch, Beijing, China; <sup>2</sup>Shimadzu (China) Co., LTD. Shanghai Branch, Shanghai, China
- MP 003 **Bioanalytical Approaches to Quantify “Free”, “Drug-bound” and “Total” Interleukin-8 in Tissue using Immuno-capture Liquid Chromatography-Mass Spectrometry;** Yue Zhao<sup>1</sup>; Huidong Gu<sup>1</sup>; Dmitry Ostanin<sup>1</sup>; Kezi Unsal-Kacmaz<sup>1</sup>; Katarzyna Urbanska<sup>1</sup>; Jianing Zeng<sup>1</sup>; Yan Zhang<sup>1</sup>; Renuka Pillutla<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb Co., Princeton, NJ
- MP 006 **Novel Highly-Specific ID-UHPLC-MS/MS Method for the Measurement of Steroid Hormones and their Conjugates in Human Serum;** Lumi Duke<sup>1</sup>; Paul H Kim<sup>2</sup>; Julianne Cook Botelho<sup>3</sup>; Candice Ulmer<sup>4</sup>; Hubert W Vesper<sup>4</sup>; <sup>1</sup>CDC Atlanta, Atlanta, GA; <sup>2</sup>Battelle Memorial Institute, Atlanta, GA 30345; <sup>3</sup>Centers for Disease Control and Prevention, Atlanta, Georgia 30341; <sup>4</sup>Centers for Disease Control and Prevention, Atlanta, Georgia
- MP 008 **In-Depth Determination of Single Amino Acid Variants in CD24+ Subpopulation of Pancreatic Cancer by nano LC-MS/MS;** Jianhui Zhu<sup>1</sup>; Zhijing Tan<sup>1</sup>; Xinpei Yi<sup>2</sup>; Jie Zhang<sup>1</sup>; David M. Lubman<sup>1</sup>; <sup>1</sup>University of Michigan Medical Center, Ann Arbor, MI; <sup>2</sup>Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing, China
- MP 012 **Integrative Proteomics Links CSF Biomarkers to Pathological Networks in the Alzheimer’s Disease Brain;** Lenora Higginbotham<sup>1</sup>; Lingyan Ping<sup>1</sup>; Eric B. Dammer<sup>1</sup>; Duc M. Duong<sup>1</sup>; Maotian Zhou<sup>1</sup>; Thomas S Wingo<sup>1</sup>; Erik C.B. Johnson<sup>1</sup>; James J. Lah<sup>1</sup>; Allan I. Levey<sup>1</sup>; Nicholas T. Seyfried<sup>1</sup>; <sup>1</sup>Emory University, Atlanta, GA
- MP 013 **Catch them Sleeping: Quick and Routine Quantification of Melatonin in Plasma with Ultivo LC/TQ;** Mark Sartain<sup>1</sup>; Aaron Boice<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA
- MP 015 **Absolute Quantitation of Non-Human Glycan (Neu5Gc)for Gastric Cancer Screening;** Nari Seo<sup>1,2</sup>; Myung Jin Oh<sup>1,2</sup>; Jaekyoung Ko<sup>1,2</sup>; Yoon Jin Choi<sup>3</sup>; Dong Ho Lee<sup>4</sup>; Hyun Joo An<sup>1,2</sup>; <sup>1</sup>Chungnam national university, Daejeon, South Korea; <sup>2</sup>Asia-Pacific Glycomics Reference Site, Daejeon, South Korea; <sup>3</sup>Department of Gastroenterology, , Korea University Guro Hospital, Seoul, South Korea; <sup>4</sup>Department of Internal Medicine, Seoul National University Bundang Hospital, Seongnam-si, South Korea
- MP 023 **Quantification of Specific Organophosphorous Pesticides, Synthetic Pyrethroids, and 2,4-Dichlorophenoxyacetic acid by LC-MS/MS;** Dickson Wambua<sup>1</sup>; Isuru Vidanage<sup>1</sup>; William Roman<sup>1</sup>; Antonia M. Calafat<sup>1</sup>; Maria Ospina<sup>1</sup>; <sup>1</sup>Centers for Disease Control and Prevention, Atlanta, Georgia 30341
- MP 024 **Development of a High-Throughput Top-Down-Proteomic Technology to Study the Associations between Apolipoprotein A-I Proteoforms and HDL Function;** Henrique Dos Santos Seckler<sup>1</sup>; John T Wilkins<sup>1</sup>; Jonathan Scott Rink<sup>2</sup>; Luca Fornelli<sup>3</sup>; Richard D Leduc<sup>1</sup>; Allan D. Sniderman<sup>4</sup>; Colby Shad Thaxton<sup>2</sup>; Donald Lloyd-Jones<sup>2</sup>; Philip D. Compton<sup>1</sup>; Neil L Kelleher<sup>1</sup>; <sup>1</sup>Northwestern University, Evanston, IL; <sup>2</sup>Northwestern University, Chicago, IL; <sup>3</sup>University of Oklahoma, Norman, OK; <sup>4</sup>McGill Centre for Translational Research in Cancer, Segal Cancer Centre / Lady Davis Institute, Jewish General Hospital, Montreal, QC
- MP 025 **An improved IonStar proteomics strategy outperforms Spectronaut in reliable quantitative analysis of large biological cohorts;** Xue Wang<sup>1</sup>; jun qu<sup>2</sup>; <sup>1</sup>University at Buffalo, Buffalo, NY; <sup>2</sup>University at Buffalo, SUNY, Buffalo, NY
- MP 028 **Fully Automated Quantitative Assessment of Methylmalonic Acid on Blood Cards Using Direct Isotope Dilution Mass Spectrometry;** Jeremiah C Jamrom<sup>1</sup>; Logan Miller<sup>1,2</sup>; Scott Faber<sup>1</sup>; John Kern<sup>1</sup>; Matt Pamuku<sup>3</sup>; Skip Kingston<sup>1</sup>; Fred D. Foster<sup>4</sup>; <sup>1</sup>Duquesne University, Pittsburgh, PA; <sup>2</sup>Shimadzu Scientific Instruments, Inc., Columbia, Maryland; <sup>3</sup>Applied Isotope Technologies, PITTSBURGH, PA; <sup>4</sup>Gerstel, Inc., Linthicum, MD



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- MP 055 **Accelerated biomolecular cross-linking by contained-electrospray ionization for rapid detection by mass spectrometry;** Benjamin J. Burris<sup>1</sup>; Abraham K. Badu-Tawiah<sup>1</sup>; <sup>1</sup>*The Ohio State University, Columbus, OH*
- MP 061 **Reducing the global burden of infectious diseases through precision infection management (PIM);** Ian Lewis<sup>1</sup>; Fiona Clement<sup>1</sup>; Deirdre L Church<sup>2</sup>; Ashlee Earl<sup>3</sup>; Yonatan Grad<sup>4</sup>; Christopher Naugler<sup>2</sup>; Sergei Noskov<sup>1</sup>; <sup>1</sup>*University of Calgary, Calgary, AB*; <sup>2</sup>*Calgary Laboratory Services, Calgary, AB*; <sup>3</sup>*Broad Institute of MIT and Harvard, Cambridge, MA*; <sup>4</sup>*Harvard T.H. Chan School of Public Health, Boston, MA*
- MP 065 **Dried Blood Spheroids for Stabilizing Acylcarnitines in Micro-liter Blood Samples Stored under Ambient Conditions;** Benji Frey<sup>1</sup>; Deidre E. Damon<sup>1</sup>; Abraham K. Badu-Tawiah<sup>1</sup>; <sup>1</sup>*The Ohio State University, Columbus, OH*
- MP 066 **Quantification of 11-plex LSD enzyme activity using LC-MS/MS;** Ryuichi Mashima<sup>1</sup>; Torayuki Okuyama<sup>1</sup>; Mari Ohira<sup>1</sup>; <sup>1</sup>*National Center for Child Health and Development, Setagaya-Ku, Japan*
- MP 071 **Fully Automated LC-MS/MS Analysis of Anticoagulants Using a Stable Isotope Labelled Internal Standards;** Toshikazu Minohata<sup>1,2</sup>; Yuki Uno<sup>2</sup>; Sigrid Baumgarten<sup>3</sup>; Stéphane Moreau<sup>3</sup>; Fanny Dayot<sup>1</sup>; Jean-François Hoeffler<sup>1</sup>; <sup>1</sup>*Alsachim SAS, Illkirch, France*; <sup>2</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>3</sup>*Shimadzu Europa GmbH, Duisburg, Germany*
- MP 072 **Sensitive Cortisol Analysis Using a Single Hair with Nanoflow UPLC- MS3 Tandem Mass Spectrometry;** Chih-Wei Chang<sup>1,2</sup>; Linjer Chen<sup>1</sup>; Li-Jung Ma<sup>1</sup>; Pin-Hsuan Wang<sup>1</sup>; Yet-Ran Chen<sup>2</sup>; Pao-Chi Liao<sup>1</sup>; <sup>1</sup>*Department of Occupational and Environmental Health, Medical College, National Cheng Kung University, Tainan, Taiwan*; <sup>2</sup>*Agriculture Biotechnology Research Center, Academia Sinica, Taipei, Taiwan*
- MP 082 **Development of glycosaminoglycan assays for mucopolysaccharidoses using LC-MS/MS;** Takanari Hattori<sup>1</sup>; Tetsuo Iida<sup>1</sup>; Jun Watanabe<sup>1</sup>; Misa Tanaka<sup>2</sup>; Hironori Kobayashi<sup>3</sup>; Shunji Tomatsu<sup>4</sup>; <sup>1</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>2</sup>*MS specialite, Yokohama, Japan*; <sup>3</sup>*Department of Pediatrics, Shimane University Faculty of Medicine, Izumo, Japan*; <sup>4</sup>*Nemours/Alfred I. duPont Hospital for Children, Wilmington, Delaware*
- MP 085 **A New Strategy Optimized for Metabolite Profiling on a Tribid Mass Spectrometer Platform;** Qian Ruan<sup>1</sup>; Kenneth P. Matuszak<sup>2</sup>; Kate J. Comstock<sup>3</sup>; <sup>1</sup>*Bristol-Myers Squibb, Princeton, NJ*; <sup>2</sup>*ThermoFisher Scientific, Bannockburn, IL*; <sup>3</sup>*ThermoFisher Scientific, San Jose, CA*
- MP 093 **Metabolism Study of Simvastatin in Rat Tissues using MALDI Orbitrap Mass Spectrometry;** Wencui Yin<sup>1</sup>; Adnan A Kadi<sup>1</sup>; Alwabli Reem<sup>1</sup>; Rahman M A f m<sup>1</sup>; <sup>1</sup>*King Saud University, Riyadh, Saudi Arabia*
- MP 094 **Ultraviolet Photodissociation Enables Confirmation of Site Specific Glucuronidation on Small Molecule Metabolites;** Joe R. Cannon<sup>1</sup>; Zhoupeng Zhang<sup>1</sup>; Joshua Nicklay<sup>2</sup>; Romain Huguet<sup>2</sup>; Scott M. Peterman<sup>2</sup>; Nichoals Duczak<sup>2</sup>; Mark Cancilla<sup>1</sup>; <sup>1</sup>*Merck & Co., Inc., West Point, PA*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*
- MP 105 **Comprehensive analysis of isoprenoid pathway intermediates and associated metabolites by HILIC-QTOF LC/MS;** Edward Baidoo<sup>1</sup>; Yuqin Dai<sup>2</sup>; Veronica Teixeira Benites<sup>1</sup>; <sup>1</sup>*Joint BioEnergy Institute/LBNL, Emeryville, CA*; <sup>2</sup>*Agilent Technologies, Santa Clara, CA*
- MP 122 **A Novel Use of Isotopomers for In Situ Calibration;** Anthony Qualley<sup>1,2</sup>; Geoffrey Hughes<sup>1,2</sup>; Thomas Malloy IV<sup>3</sup>; Ted Piatkowski<sup>3</sup>; Benjamin A Clapp<sup>2</sup>; H. Mitchell Rubenstein<sup>2</sup>; <sup>1</sup>*UES, Inc., Dayton, OH*; <sup>2</sup>*USAF-AFRL, WPAFB, OH*; <sup>3</sup>*Batelle, Columbus, OH*
- MP 123 **Characterization of arsenic metabolites and protein-binding using chromatography coupled to multiple mass spectrometry techniques;** Hanyong Peng<sup>1</sup>; Bin Hu<sup>2</sup>; Qingqing Liu<sup>1</sup>; Xiufen Lu<sup>1</sup>; Xiaowen Yan<sup>1</sup>; X. Chris Le<sup>3</sup>; <sup>1</sup>*University of Alberta, Edmonton*; <sup>2</sup>*Wuhan University, Wuhan, China*; <sup>3</sup>*University of Alberta, Edmonton, AB*
- MP 128 **Tracking Microcystin Oxidation Product Formation by Liquid Chromatography/High Resolution Mass Spectrometry (LC/HRMS) and Implications for Process Monitoring and Treatment;** Judy Westrick<sup>1</sup>;



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- Johnna A Birbeck<sup>1</sup>; Nicholas Peraino<sup>1</sup>; David C Szlag<sup>2</sup>; <sup>1</sup>Wayne State University, Detroit, MI; <sup>2</sup>Oakland University, Rochester, MI
- MP 139 **Analysis of Dioxins Utilizing Time-of-Flight for Low Level Quantitation;** Tim Conjelko<sup>1</sup>; Courtney Milner<sup>1</sup>; Jeff Hollis<sup>1</sup>; Matthew Curtis<sup>1</sup>; <sup>1</sup>Agilent Technologies, Inc., Santa Clara, CA
- MP 143 **Short Chain Chlorinated Paraffins (SCCPs) analysis using negative chemical ionization (CI) and low energy EI by high-resolution GC/Q-TOF;** Sofia Nieto<sup>1</sup>; Matthew Curtis<sup>1</sup>; Nathan Eno<sup>1</sup>; Courtney Milner<sup>1</sup>; Pierre Dumas<sup>2</sup>; <sup>1</sup>Agilent Technologies, Inc., Santa Clara, CA; <sup>2</sup>Institut National de Santé Publique du Québec (INSPQ), Québec, QC
- MP 144 **Analysis of the wastewater effluent samples to identify toxic chemicals using high-resolution GC/Q-TOF;** Sofia Nieto<sup>1</sup>; Kai Chen<sup>1</sup>; Courtney Milner<sup>1</sup>; Thomas Young<sup>2</sup>; <sup>1</sup>Agilent Technologies, Inc., Santa Clara, CA; <sup>2</sup>University of California, Davis, Davis, CA
- MP 148 **How is ?-cyclocitral formed in SPME GC/MS of a cyanobacterium?;** Ryuji Yamashita<sup>1</sup>; Keisuke Kanei<sup>1</sup>; Eri Yamauchi<sup>1</sup>; Koji Tomita<sup>2</sup>; Kiyomi Tsuji<sup>3</sup>; Ken-ichi Harada<sup>1</sup>; <sup>1</sup>Meijo University, Nagoya, Japan; <sup>2</sup>Aichi Prefectural Institute of Public Health, Nagoya, Japan; <sup>3</sup>Kanagawa Prefectural Institute of Public Health, Chigasaki, Japan
- MP 164 **Dynamics of histone H3.3K27me3 in pluripotency and differentiation of embryonic stem cells revealed by stable isotope labeling mass spectrometry;** Yekaterina Kori<sup>1</sup>; Simone Sidoli<sup>1</sup>; Zuo-Fei Yuan<sup>2</sup>; Benjamin A. Garcia<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA; <sup>2</sup>University of Pennsylvania, Philadelphia, PA
- MP 167 **Understanding epigenome and proteome remodeling caused by novel germline histone H3.3 mutations during neurodevelopment;** Khadija D Wilson<sup>1</sup>; Geoffrey P. Dann<sup>1</sup>; Elizabeth J. Bhoj<sup>2</sup>; Hakon H Hakonarson<sup>2</sup>; Benjamin A. Garcia<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA; <sup>2</sup>Children's Hospital of Philadelphia, Philadelphia, PA
- MP 170 **Inhibition of Kinases Reveals Distant Links Between Signaling Pathways and the Histone Code;** Kevin A. Janssen<sup>1</sup>; Laura M. Agosto<sup>1</sup>; Benjamin A. Garcia<sup>1</sup>; <sup>1</sup>Perelman School of Medicine - University of Pennsylvania, Philadelphia, PA
- MP 174 **Novel UHPLC-MRM-MS approach allows for absolute quantification of histone PTMs in as little as 20 minutes;** Joseph Cesare<sup>1</sup>; Zuofei Yuan<sup>1</sup>; Steven Zhao<sup>1</sup>; Peder Lund<sup>1</sup>; Josue Baeza<sup>1</sup>; Yekaterina Kori<sup>1</sup>; Simone Sidoli<sup>1</sup>; Hee Jong Kim<sup>1</sup>; Hyoungjoo Lee<sup>1</sup>; Kathryn E. Wellen<sup>1</sup>; Benjamin A. Garcia<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA
- MP 181 **EU compliant routine quantitative dioxin, dioxin-like PCB and marker PCB analysis by GC-MS/MS using an advanced electron ionisation source;** Dominic Roberts<sup>1</sup>; Alexander Schachtele<sup>2</sup>; Richard Law<sup>3</sup>; Tim Anderson<sup>4</sup>; Adam Ladak<sup>4</sup>; Cristian Cojocariu<sup>3</sup>; <sup>1</sup>Thermo Fisher Scientific, Runcorn, United Kingdom; <sup>2</sup>European Union Reference Laboratory for halogenated POPs in feed and food, Freiburg, Germany; <sup>3</sup>Thermo Fisher Scientific, TUDOR ROAD, United Kingdom; <sup>4</sup>Thermo Fisher Scientific, Austin, Texas
- MP 188 **High Throughput Target and Suspect Pesticide Analysis using a new LC/Q-TOF Screener Software;** Karen E Yannell<sup>1</sup>; Kai Chen<sup>2</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>Agilent Technologies, Inc., Santa Clara, CA
- MP 190 **Analysis of Patulin in Fruit Juices and Extracts Using Liquid Chromatography Triple Quadrupole Mass Spectrometry;** Claudia P.B. Martins<sup>1</sup>; Cristina C. Jacob<sup>1</sup>; Michael Volny<sup>1</sup>; Mary L. Blackburn<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA
- MP 191 **A Fast, Sensitive and Comprehensive Assay to Quantify Pesticide Residues in Dietary Supplements using GC/MS/MS coupled with QuEChERS Extraction Method;** Aihua Liu<sup>1</sup>; Abhijit Ghosh<sup>1</sup>; Spencer Carter<sup>1</sup>; <sup>1</sup>Dyad Labs, Salt Lake City, UT
- MP 195 **Development and Validation of a new sensitive and rapid UPLC-MS-MS method to determine acrylamide in coffee;** Yilong Zheng<sup>1</sup>; Zhitian Zhang<sup>1</sup>; Jillian O'connell<sup>1</sup>; Junsuo Li<sup>1</sup>; <sup>1</sup>Intertek, Champaign, IL



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- MP 198 **Off-flavor system of Shimadzu analyzes the odor components in edible oil;** Liu Xiaohua; *Shimadzu (China) Co., Ltd., Guangzhou, China*
- MP 204 **Assessing Peptide Profiling Reproducibility of Single Source Human Head Hair ;** Maria Lawas<sup>1</sup>; Katherine F. Jones<sup>1</sup>; Katelyn E. Mason<sup>2</sup>; Deon S. Anex<sup>2</sup>; Traci L. Carlson<sup>1</sup>; Luisa V. Forger<sup>1</sup>; Brian A. Eckenrode<sup>3</sup>; Bradley Hart<sup>2</sup>; Joseph Donfack<sup>3</sup>; <sup>1</sup>*Counterterrorism and Forensic Science Research Unit, Visiting Scientist Program, Federal Bureau of Investigation Laboratory Division, Quantico, VA*; <sup>2</sup>*Forensic Science Center, Lawrence Livermore National Laboratory, Livermore, CA*; <sup>3</sup>*Counterterrorism and Forensic Science Research Unit, Federal Bureau of Investigation Laboratory Division, Quantico, VA*
- MP 210 **Identification of human haemoglobin variants through advanced forensic mass spectrometry of blood;** Cameron Heaton<sup>1</sup>; Laura Cole<sup>1</sup>; Richard R McColm<sup>2</sup>; Jason Eyre<sup>3</sup>; Simona Francese<sup>1</sup>; <sup>1</sup>*BMRC, Sheffield Hallam University, Sheffield, United Kingdom*; <sup>2</sup>*DSTL, Porton Down, Salisbury, United Kingdom*; <sup>3</sup>*BMS Haemolysis Lab, Haematology Department, Sheffield Teaching Hospital, Sheffield, United Kingdom*
- MP 213 **A method for Simultaneous Targeted and Non-Targeted LC-HRMS/MS Drug Screening in Forensic Toxicology;** Jason E Schaff<sup>1</sup>; Preston C Lowe<sup>1</sup>; Madeline A Montgomery<sup>1</sup>; Cynthia L Morris-Kukoski<sup>1</sup>; <sup>1</sup>*FBI Laboratory Chem Unit, Quantico, VA*
- MP 215 **Thread Spray Mass Spectrometry for Direct Analysis of Hemoglobin in Whole Blood;** Sierra Jackson<sup>1</sup>; Abraham K. Badu-Tawiah<sup>1</sup>; <sup>1</sup>*The Ohio State University, Columbus, OH*
- MP 218 **Use of IRMPD Spectroscopy to Characterize Derivatives of Aldehydes Considered Emerging Explosive Threat Compounds;** Connor J Graca<sup>1</sup>; Luke Metzler<sup>1</sup>; Theodore Corcovilos<sup>1</sup>; Giel Berden<sup>2</sup>; Jonathan Martens<sup>2</sup>; Jos Oomens<sup>2, 3</sup>; Michael Van Stipdonk<sup>1</sup>; <sup>1</sup>*Duquesne University, Pittsburgh, PA*; <sup>2</sup>*Radboud University Nijmegen, Institute for Molecules and Materials, FELIX Facility, Nijmegen, Netherlands*; <sup>3</sup>*University of Amsterdam, Amsterdam, Netherlands*
- MP 222 **Analysis of Cosmetic Products for Evidentiary Value via Paper Spray and Paper Cone Spray Ionization-Mass Spectrometry;** Abigail M. Poehls<sup>1</sup>; Shahnaz Mukta<sup>1</sup>; Christopher C. Mulligan<sup>1</sup>; <sup>1</sup>*Illinois State University, Normal, IL*
- MP 223 **Rapid Profiling of Authentic Forensic Evidence via Paper Cone Spray Ionization Employed on Portable MS Instrumentation;** Ashley R. Stelmack<sup>1</sup>; William L. Fatigante<sup>1</sup>; Shahnaz Mukta<sup>1</sup>; Christopher C. Mulligan<sup>2</sup>; <sup>1</sup>*Illinois state university, Normal, IL*; <sup>2</sup>*Illinois State University, Normal, IL*
- MP 224 **The Performance of Nanoparticle-Modified Paper Substrates Employed as Surface Transfer Swabs for Combined SERS and PSI-MS Investigation;** Trevor J. McDaniel<sup>1</sup>; Noah W. McClurg<sup>1</sup>; William L. Fatigante<sup>1</sup>; Jun-Hyun Kim<sup>1</sup>; Jeremy D. Driskell<sup>1</sup>; Christopher Mulligan<sup>2</sup>; <sup>1</sup>*Illinois state university, Normal, IL*; <sup>2</sup>*Illinois State University, Normal, IL*
- MP 242 **Isomeric ?-Carbon- and ?-Centered Glycylglycyltryptophan Radical Cations and their Dissociation Product Ions: Structural, Energetic, Mechanistic, and Spectroscopic Investigations;** Mengzhu Li<sup>1</sup>; Yinan Li<sup>1</sup>; Chi Kit Andy Siu<sup>2</sup>; Jonathan Martens<sup>3</sup>; Jos Oomens<sup>3</sup>; Keung Ivan Chu<sup>2</sup>; <sup>1</sup>*Department of Chemistry, The University of Hong Kong, Hong Kong, Hong Kong*; <sup>2</sup>*Department of Chemistry, City University of Hong Kong, Hong Kong, Hong Kong*; <sup>3</sup>*FELIX Laboratory, Institute for Molecules and Materials, Nijmegen, Netherlands*
- MP 246 **Novel C?-C? Cleavage of N-terminal Phenylalanine Residues of Tyrosine-Containing Peptide Radical Cations: Structural, Mechanistic, and Photodissociation Spectroscopic Investigations;** Wai Kit Tang<sup>1</sup>; Xiaoyan Mu<sup>2</sup>; Naiping Dong<sup>2</sup>; Jonathan Martens<sup>3</sup>; Daniel Michael Spencer<sup>2</sup>; Mengzhu Li<sup>2</sup>; Jos Oomens<sup>3</sup>; Chi Kit Andy Siu<sup>1</sup>; Ivan K. Chu<sup>4</sup>; <sup>1</sup>*Department of Chemistry, City University of Hong Kong, Hong Kong, Hong Kong*; <sup>2</sup>*Department of Chemistry, University of Hong Kong, Hong Kong, Hong Kong*; <sup>3</sup>*FELIX Laboratory, Institute for Molecules and Materials, Nijmegen, Netherlands*; <sup>4</sup>*University of Hong Kong, Hong Kong, Hong Kong*



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- MP 252 **An Orthoester Derivatization Strategy for the Structure Elucidation of Vicinal Diols;** Renzo A Samame<sup>1</sup>; Chengli Zu<sup>1</sup>; Daniel Knueppel<sup>1</sup>; Jeffery Gilbert<sup>1</sup>; <sup>1</sup>*Corteva Agriscience, Indianapolis, IN*
- MP 262 **Gas-phase photodissociative crosslinking of diazirine-modified adrenaline with the binding motif of beta-2 adrenergic receptor;** Yang Liu<sup>1</sup>; Shu R. Huang<sup>1</sup>; Frantisek Turecek<sup>1</sup>; <sup>1</sup>*University of Washington, Seattle, WA*
- MP 263 **Thermochemistry of the Ion-Molecule Reactions of Uranium Fluoride Species by Guided Ion Beam Tandem Mass Spectrometry;** Amanda Bubas<sup>1</sup>; Cameron J. Owen<sup>1</sup>; Peter B. Armentrout<sup>1</sup>; <sup>1</sup>*University of Utah, Salt Lake City, UT*
- MP 270 **Automated UV Action Spectroscopy on a Modified 3D Ion Trap MS for Structural Analysis of DNA Cation-Radicals;** Andy Dang<sup>1</sup>; James Gladden<sup>1</sup>; Yue Liu<sup>1</sup>; Brandon Mozzone<sup>1</sup>; Frantisek Turecek<sup>1</sup>; <sup>1</sup>*University of Washington, Seattle, WA*
- MP 272 **Measurement of the Asymmetric UO22+ Stretching Frequency for [UVIO2(X)3]- (X = F, Cl, Br and I) Species Using IRMPD Spectroscopy;** Irena Tatosian<sup>1</sup>; Luke Metzler<sup>1</sup>; Connor J Graca<sup>1</sup>; Theodore Corcovilos<sup>1</sup>; Jonathan Martens<sup>2</sup>; Giel Berden<sup>2</sup>; Jos Oomens<sup>2</sup>; Michael Van Stipdonk<sup>1</sup>; <sup>1</sup>*Duquesne University, Pittsburgh, PA*; <sup>2</sup>*Radboud University Nijmegen, Institute for Molecules and Materials, FELIX Facility, Nijmegen, Netherlands*
- MP 281 **Decarboxylative coupling reactions catalyzed by first-row transition metal complexes with crown ether;** Elettra L. Piacentino<sup>1</sup>; Fotis Pappas Pappas<sup>2</sup>; Kostantinos Pappas<sup>2</sup>; Michael Lesslie<sup>2</sup>; Thomas M. Gilbert<sup>2</sup>; Richard A. J. O'hair<sup>3</sup>; Victor Ryzhov<sup>2</sup>; <sup>1</sup>*Northern Illinois University, DeKalb*; <sup>2</sup>*Northern Illinois University, DeKalb, IL*; <sup>3</sup>*University of Melbourne, Melbourne, Australia*
- MP 282 **Gas-Phase Study of C-N Coupling Reactions Catalyzed by Transition Metal Complexes;** Kevin E Parker<sup>1</sup>; Victor Ryzhov<sup>2</sup>; <sup>1</sup>*Northern Illinois University, DeKalb, IL*; <sup>2</sup>*Northern Illinois University, DeKalb, IL*
- MP 292 **Thin film dialysis HX-MS reveals protein interfaces during reversible self-association of monoclonal antibodies at high concentration;** Mihiri Weerasinghe<sup>1</sup>; Yangjie Wei<sup>2</sup>; Reza Esfandiary<sup>3</sup>; C. Russell Middaugh<sup>2</sup>; David D Weis<sup>1,4</sup>; <sup>1</sup>*Department of Chemistry, University of Kansas, Lawrence, Kansas (KS)*; <sup>2</sup>*Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, Kansas (KS)*; <sup>3</sup>*Department of Formulation Sciences, MedImmune LLC, Gaithersburg, MD*; <sup>4</sup>*Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, Kansas (KS)*
- MP 294 **A Comparison between Two Automated HDXMS Systems, as Applied to Epitope Mapping;** Aik Roy Heng<sup>1</sup>; Deepa Balasubramaniam<sup>1</sup>; Jonathan Fitchett<sup>1</sup>; Ruben Haro<sup>2</sup>; Michael J. Chalmers<sup>3</sup>; <sup>1</sup>*Lilly Biotechnology Center, San Diego, CA*; <sup>2</sup>*Discovery Automation, Centro de Investigación, Alcobendas, Spain*; <sup>3</sup>*Lilly Research Laboratories, Eli Lilly and Company, Indianapolis, IN*
- MP 298 **HDX-MS as a tool for probing conformational stability in industrial applications;** Daniel W Pedersen<sup>1,2</sup>; Jeppe C Mouritsen<sup>1</sup>; Christian I Jørgensen<sup>1</sup>; Thomas J D Jørgensen<sup>2</sup>; <sup>1</sup>*Novozymes A/S, Bagsværd, Denmark*; <sup>2</sup>*University of Southern Denmark, Odense, Denmark*
- MP 300 **Integrated software platform for analyzing hydrogen-deuterium exchange and oxidative footprinting data for solvent accessibility;** Wilfred Tang<sup>1</sup>; Marshall Bern<sup>1</sup>; Rose D Lawler<sup>1</sup>; Yong J. Kil<sup>1</sup>; Eric Carlson<sup>1</sup>; Saketh Chemuru<sup>2</sup>; Nicole D Wagner<sup>2</sup>; Liuqing Shi<sup>2</sup>; Henry Rohrs<sup>2</sup>; Daisy W. Leung<sup>2</sup>; Michael L Gross<sup>2</sup>; <sup>1</sup>*Protein Metrics Inc., Cupertino, CA*; <sup>2</sup>*Washington University, St. Louis, MO*
- MP 309 **20S Proteasome Complex Structure Conformation and Dynamics Study by Hydrogen Deuterium Exchange Mass Spectrometry;** Shaunak Paval<sup>1</sup>; Terry Zhang<sup>2</sup>; Rosa Viner<sup>3</sup>; Albert Konijnenberg<sup>4</sup>; David C Schriemer<sup>1</sup>; Andreas Huhmer<sup>3</sup>; <sup>1</sup>*University of Calgary, Calgary, AB*; <sup>2</sup>*ThermoFisher, San Jose, CA*; <sup>3</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>4</sup>*Thermo Fisher Scientific, Eindhoven, Netherlands*
- MP 320 **Extractables & Leachables Analysis using the Hi-Resolution Accurate Mass GC/QTOF;** Thomas S Talwar<sup>1</sup>; Matthew Curtis<sup>2</sup>; <sup>1</sup>*Agilent Technologies, Inc., Wilmington, DE*; <sup>2</sup>*Agilent Technologies, Inc., Santa Clara, CA*



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- MP 327 **Using TOF-MS to Improve Quality in High Throughput Laboratories;** Lucas Marshall<sup>1</sup>; Jason Hull, MS<sup>1</sup>; Rebecca Heltsley, PhD<sup>1</sup>; <sup>1</sup>*Aegis Sciences Corporation, Nashville, TN*
- MP 341 **Co-Registered MALDI and ToF-SIMS Data for Visualizing Sub-cellular Signaling Pathways in the Brain;** Matthias Lorenz<sup>1</sup>; Stephen T. King<sup>1</sup>; Chad A. Steed<sup>1</sup>; Junghoon Chae<sup>1</sup>; Anton V. Ievlev<sup>1</sup>; Olga S. Ovchinnikova<sup>1</sup>; <sup>1</sup>*Oak Ridge National Laboratory, Oak Ridge, TN*
- MP 360 **A Quantitative Evaluation of Ion Chromatogram Extraction Algorithms;** Annika Tostengard<sup>1</sup>; Robert Smith<sup>2</sup>; <sup>1</sup>*The University of Montana, Missoula, MT*; <sup>2</sup>*University of Montana Missoula, Missoula, MT*
- MP 388 **Bonfire Search Engine for Precursor-Independent Identification of Peptides with Exact or Open Modification to Uncover the “Dark Proteome”;** Wen Yu<sup>1</sup>; Raghothama Chaerkady<sup>1</sup>; Xiaotao Qu<sup>1</sup>; Sonja Hess<sup>1</sup>; David A Fenstermacher<sup>1</sup>; <sup>1</sup>*MedImmune, Gaithersburg, MD*
- MP 396 **Ion mobility enhanced matching between LC-MS runs and collisional cross section prediction improve identification and quantification in MaxQuant;** Nikita Prianichnikov<sup>1</sup>; Favio Salinas Soto<sup>1</sup>; Heiner Koch<sup>2</sup>; Scarlet Koch<sup>2</sup>; Markus Lubeck<sup>2</sup>; Sven Brehmer<sup>2</sup>; Juergen Cox<sup>1</sup>; <sup>1</sup>*Max Planck Institute of Biochemistry, Martinsried, Germany*; <sup>2</sup>*Bruker Daltonik GmbH, Bremen, Germany*
- MP 398 **Automating distributed analysis of large MS/MS datasets;** Julie S Wertz<sup>1</sup>; Jeremy Carver<sup>1</sup>; Nuno Bandeira<sup>1</sup>; <sup>1</sup>*University of California San Diego, La Jolla, CA*
- MP 401 **Bolt: A new age peptide search engine for comprehensive MS/MS sequencing through vast protein databases in minutes;** Amol Prakash<sup>1</sup>; Swetaketu Majumder<sup>1</sup>; Shadab Ahmad<sup>1</sup>; Conor Jenkins<sup>2</sup>; Benjamin Orsburn<sup>3</sup>; <sup>1</sup>*Optys Tech Corporation, Shrewsbury, MA*; <sup>2</sup>*Hood College Bioinformatics Program, Frederick, MD*; <sup>3</sup>*National Cancer Institute @ Frederick, Frederick, MD*
- MP 411 **Parametric Model Selection Methods for Estimating Target and Decoy Distributions using Mass Spectrum Characteristics;** Benjamin A. Stark<sup>1</sup>; Robert Smith<sup>1</sup>; <sup>1</sup>*University of Montana, Missoula, MT*
- MP 414 **Optimizing the isolation width in Orbitrap instruments to maximize the number of label-free quantified peptides and protein;** Carmen Paschke<sup>1</sup>; Waqas Nasir<sup>1</sup>; Kai Fritzscheier<sup>1</sup>; Rosa Rakownikow Jersie-Christensen<sup>1</sup>; Tabiwang N. Arrey<sup>1</sup>; David Horn<sup>2</sup>; Martin Zeller<sup>1</sup>; Romain Huguet<sup>2</sup>; Bernard Delanghe<sup>3</sup>; <sup>1</sup>*Thermo Fisher Scientific, Bremen, Germany*; <sup>2</sup>*ThermoFisher, San Jose, CA*; <sup>3</sup>*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*
- MP 416 **FragPipe: a fast proteomics pipeline with MSFragger search engine at heart;** Dmitry Avtonomov<sup>1</sup>; Andy T. Kong<sup>1</sup>; Felipe V. Leprevost<sup>1</sup>; Guo-Ci Teo<sup>1</sup>; Hui-yin Chang<sup>1</sup>; Alexey I. Nesvizhskii<sup>1</sup>; <sup>1</sup>*University of Michigan, Ann Arbor, MI*
- MP 421 **Assessing the validity of protein inference on a large environmental metaproteomic dataset - ProteOMZ Expedition of the Central Pacific Ocean;** Jaclyn K. Saunders<sup>1</sup>; Matthew McIlvin<sup>1</sup>; Dawn Moran<sup>1</sup>; Noelle Held<sup>1</sup>; Chris Dupont<sup>2</sup>; Alyson Santoro<sup>3</sup>; Mak Saito<sup>1</sup>; <sup>1</sup>*Woods Hole Oceanographic Institution, Woods Hole, MA*; <sup>2</sup>*J. Craig Venter Institute, La Jolla, CA*; <sup>3</sup>*University of California, Santa Barbara, Santa Barbara, CA*
- MP 422 **Propagating uncertainty in protein-level quantifications is key to robust downstream analysis of bottom-up proteomics data;** Alexander Phillips<sup>1</sup>; Ranjeet S Bhamber<sup>2</sup>; Anna Tierney<sup>3</sup>; Martin Rusilowicz<sup>3</sup>; Simon Maskell<sup>1</sup>; Simon Hubbard<sup>3</sup>; Andrew R Jones<sup>1</sup>; Richard Unwin<sup>3</sup>; Andrew W Dowsey<sup>2</sup>; <sup>1</sup>*University of Liverpool, Liverpool, United Kingdom*; <sup>2</sup>*University of Bristol, Bristol, United Kingdom*; <sup>3</sup>*University of Manchester, Manchester, United Kingdom*
- MP 429 **A Platform Approach to Managing Developability and Manufacturability Assessments of Biotherapeutics;** Albert Van Wyk<sup>1</sup>; Joe Shambaugh<sup>2</sup>; John McCarter<sup>2</sup>; Aude Tartiere<sup>3</sup>; Christopher Smith<sup>2</sup>; Amanda Fitzgerald<sup>2</sup>; Cassandra Wigmore<sup>4</sup>; Peter Haber<sup>5</sup>; <sup>1</sup>*Genedata Ltd, Cambridge, United Kingdom*; <sup>2</sup>*Genedata, Inc., Lexington, MA*; <sup>3</sup>*Genedata, Inc., San Francisco, CA*; <sup>4</sup>*Genedata AG, Basel, Switzerland*; <sup>5</sup>*Genedata GmbH, Munich, Germany*



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- MP 434 **Implementing a generic scripting node to a standard proteomics workflow processing software;** Frank Berg<sup>1</sup>; Kai Fritzscheier<sup>1</sup>; Carmen Paschke<sup>1</sup>; Torsten Ueckert<sup>1</sup>; David Horn<sup>2</sup>; Bernard Delanghe<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, Bremen, Germany*; <sup>2</sup>*ThermoFisher, San Jose, CA*
- MP 435 **Simple interface web application for biomaker validation;** Jaenyeon Kim<sup>1</sup>; Hyunsoo Kim<sup>2</sup>; Injoon Yeo<sup>3</sup>; Areum Sohn<sup>2</sup>; Youngsoo Kim<sup>2,3,4</sup>; <sup>1</sup>*Seoul National University, Seoul, South Korea*; <sup>2</sup>*Seoul National University College of Medicine, Seoul, South Korea*; <sup>3</sup>*Seoul national university, Seoul, South Korea*; <sup>4</sup>*Seoul National University Hospital, Seoul, South Korea*
- MP 452 **Intra-well Imaging of Fluid Meniscus and Mass Spectra via Acoustic Mist Ionization Mass Spectrometry;** Eric Hall<sup>1</sup>; Lucien Ghislain<sup>1</sup>; Yi-wen Huang<sup>1</sup>; Sammy S Datwani<sup>1</sup>; <sup>1</sup>*Labcyte Inc., San Jose, CA*
- MP 460 **Surface effects in droplet chemistry revealed by transmission-mode liquid desorption electrospray ionization;** Taghi Sahraeian<sup>1</sup>; Dmytro Kulyk<sup>1</sup>; Abraham K. Badu-Tawiah<sup>1</sup>; <sup>1</sup>*The Ohio State University, Columbus, OH*
- MP 464 **Next Generation Sample Introduction for High-Throughput Mass Spectrometry: Acoustic Droplet Ejection with an Open Port Probe;** Lucien Ghislain<sup>1</sup>; Chang Liu<sup>2</sup>; Hui Zhang<sup>3</sup>; Jianjua Liu<sup>4</sup>; Wenyi Hua<sup>3</sup>; Timothy Foley<sup>3</sup>; Don W. Arnold<sup>5</sup>; Thomas R. Covey<sup>2</sup>; Sammy S. Datwani<sup>6</sup>; <sup>1</sup>*Labcyte Inc, San Jose, CA*; <sup>2</sup>*SCIEX, Concord, ON*; <sup>3</sup>*Pfizer, Groton, CT*; <sup>4</sup>*Pfizer Inc., Groton, CT*; <sup>5</sup>*SCIEX, Redwood Shores, CA*; <sup>6</sup>*Labcyte Inc., San Jose, CA*
- MP 466 **Spray-Capillary: An Electrohydrodynamic Spray-Assisted Device for Quantitative Ultra-Low Volume Extraction;** Lushuang Huang<sup>1</sup>; Zhe Wang<sup>1</sup>; Si Wu<sup>1</sup>; <sup>1</sup>*University of Oklahoma, Norman, OK*
- MP 475 **Optimization of the ions trajectories in a dynamically harmonized Fourier-Transform Ion Cyclotron Resonance cell using a Design of Experiments strategy;** Julien Maillard<sup>1,2</sup>; Justine Ferey<sup>1</sup>; Isabelle Schmitz-Afonso<sup>1</sup>; Soumeiya Bekri<sup>3</sup>; Thomas Gautier<sup>2</sup>; Nathalie Carrasco<sup>2</sup>; Carlos Afonso<sup>1</sup>; Abdellah Tebani<sup>3</sup>; <sup>1</sup>*Université de Rouen, Laboratoire COBRA UMR 6014 & FR 3038, IRCOF, Mont St Aignan Cedex, France*; <sup>2</sup>*LATMOS/IPSL, Université Versailles St Quentin, UPMC Université Paris 06, CNRS, Guyancourt, France*; <sup>3</sup>*Department of Metabolic Biochemistry, Rouen University Hospital, Rouen, France*
- MP 478 **Application of CAN bus in mass spectrometer design;** Ming Li<sup>1</sup>; Kai Li<sup>1</sup>; Xingbin Tang<sup>1</sup>; <sup>1</sup>*NCS Testing Technology Co., Ltd, Beijing, China*
- MP 491 **Recent Development in Improving the Precision of Quantitative Analysis for Linear Ion Trap(LIT) and LIT-Orbitrap Tandem Mass Spectrometry;** Linfan Li<sup>1</sup>; Taoqing Wang<sup>2</sup>; Anyin Li<sup>2</sup>; Jae C Schwartz<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*University of New Hampshire, Durham, NH*
- MP 494 **High Throughput Charge Detection Mass Spectrometry;** Daniel Botamanenko<sup>1</sup>; Aaron R. Todd<sup>1</sup>; Martin F Jarrold<sup>1</sup>; <sup>1</sup>*Indiana University, Bloomington, IN*
- MP 505 **A New Lipidomics Software Workflow Demonstrates Disrupted Lipogenesis Induced with Drug Treatment in Leukemia Cells;** Mark Sartain<sup>1</sup>; Genevieve Van de Bittner<sup>1</sup>; Xiangdong Li<sup>1</sup>; Jeremy Koelmel<sup>2</sup>; Adithya Murali<sup>1</sup>; Sarah Stow<sup>1</sup>; <sup>1</sup>*Agilent Technologies, Santa Clara, CA*; <sup>2</sup>*Department of Chemistry, University of Florida, Gainesville, FL*
- MP 507 **Lipid Profiling of Malaria Samples Using Orbitrap Velos Pro Mass Spectrometer with SimLipid Software;** Ningombam Sanjib Meitei<sup>1,2</sup>; Himani Gupta<sup>2</sup>; Fatima Rahlouni<sup>3</sup>; David J. Sullivan<sup>4</sup>; Vladimir Shulaev<sup>3</sup>; <sup>1</sup>*PREMIER Biosoft, Palo Alto,, CA*; <sup>2</sup>*PREMIER Biosoft, Indore, India*; <sup>3</sup>*University of North Texas, Denton, TX*; <sup>4</sup>*Bloomberg School of Public Health, Johns Hopkins University, Baltimore, MD*
- MP 511 **Untargeted Lipidomic Profiling of Bis(monoacylglycerol)phosphate Lipids in Cancer Cells and Tumor Tissues Point to Transformation Specific Regulation of Acyl Chains;** Megan Showalter<sup>1</sup>; Anastasia Berg<sup>2</sup>; Michael Sa<sup>1</sup>; Hiroshi Tsugawa<sup>3</sup>; Tobias Kind<sup>1</sup>; Kermit Carraway, III<sup>2</sup>; Oliver Fiehn<sup>1</sup>; <sup>1</sup>*UC Davis West Coast Metabolomics Center, Davis, CA*; <sup>2</sup>*Department of Biochemistry and Molecular Medicine UC Davis, Sacramento, CA*; <sup>3</sup>*RIKEN Center for Sustainable Resource Science, Wako, Japan*



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- MP 524 **Mapping the Lipid Transducers of Exercise in Rats and Human Subjects;** David Gaul<sup>1</sup>; Sam Moore<sup>1</sup>; Alexandra Coomes<sup>2</sup>; Collin Douglas<sup>2</sup>; Karyn Esser<sup>2</sup>; Neil Johannsen<sup>3</sup>; Kate Early<sup>4</sup>; <sup>1</sup>*Georgia Institute of Technology, Atlanta, GA*; <sup>2</sup>*University of Florida, Gainesville, FL*; <sup>3</sup>*Louisiana State University, Baton Rouge, LA*; <sup>4</sup>*Columbus State University, Columbus, GA*
- MP 527 **Rapid and sensitive characterization of FAHFA lipids using an untargeted lipidomics approach;** Tong Shen<sup>1</sup>; Bryan Roberts<sup>1</sup>; Oliver Fiehn<sup>1</sup>; <sup>1</sup>*UC Davis West Coast Metabolomics Center, Davis, CA*
- MP 529 **Effects of Various Temperature Related Storage Conditions on Human Plasma and Serum Lipid Profile;** Greg B Reis<sup>1</sup>; Jon Rees<sup>1</sup>; Zsuzsanna Kuklenyik<sup>1</sup>; <sup>1</sup>*Centers for Disease Control and Prevention, Atlanta, Georgia*
- MP 532 **Ion suppressing contaminants generated by multiple injections from the same sample vial negatively impact reverse phase based-lipidomics experiments;** Peter Benke<sup>1</sup>; Bo Burla<sup>1</sup>; Kim Ekroos<sup>2</sup>; Markus R Wenk<sup>1</sup>; Federico Torta<sup>1</sup>; <sup>1</sup>*National University of Singapore, Singapore, Singapore*; <sup>2</sup>*Lipidomics Consulting Ltd, Esbo, Finland*
- MP 534 **High-throughput Targeted Lipidomics Analysis of Dihydroceramide Desaturase-1 (DES1) Knockout Mice;** Mackenzie Pearson<sup>1</sup>; Santosh Kapil<sup>1</sup>; Trevor S Tippetts<sup>2</sup>; Scott A Summers<sup>2</sup>; <sup>1</sup>*Sciex, Redwood City, CA*; <sup>2</sup>*University of Utah, Salt Lake City, UT*
- MP 540 **Quantifying the lipidome for respiratory disease: A rapid and comprehensive HILIC-based targeted approach;** Giorgis Isaac<sup>1</sup>; Nyasha Munjoma<sup>2</sup>; Lee A Gethings<sup>2</sup>; Robert S Plumb<sup>1</sup>; <sup>1</sup>*Waters Corporation, Milford, MA*; <sup>2</sup>*Waters Corporation, Wilmslow, United Kingdom*
- MP 551 **Fast Supercritical Fluid Chromatography Separation and Shotgun Lipidomics with High Resolution Mass Spectrometry for the Study of Breast Cancer Metastasis;** Sheher Mohsin<sup>1</sup>; Ningombam Sanjib Meitei<sup>2</sup>; Peter Siegel<sup>3</sup>; Daina Avizonis<sup>4</sup>; Gaelle Bridon<sup>5</sup>; <sup>1</sup>*Agilent Technologies, Schaumburg, IL*; <sup>2</sup>*PREMIER Biosoft, Indore, India*; <sup>3</sup>*Goodman Cancer Research Centre, Montreal, QC*; <sup>4</sup>*Goodman Cancer Research Centre, Quebec, Montreal, Canada*; <sup>5</sup>*Agilent Technologies, Inc., Wilmington, DE*
- MP 573 **Off-line fractionation of complex samples to improve depth-of-coverage and aid compound identification in metabolomics;** Charles R Evans<sup>1</sup>; Brady G Anderson<sup>1</sup>; Maureen T Kachman<sup>1</sup>; <sup>1</sup>*University of Michigan, Ann Arbor, MI*
- MP 583 **Structural Characterization of Cyclic Peptides using a Quadrupole Time-of-Flight Mass Spectrometer;** Toshiya Matsubara<sup>1</sup>; Yusuke Inohana<sup>1</sup>; Ichiro Hirano<sup>1</sup>; <sup>1</sup>*Shimadzu Corporation, Kyoto, Japan*
- MP 589 **Increasing the Analysis Depth of the HLA-Associated Peptide Repertoire by LC-MS/MS;** Chris D McGann<sup>1</sup>; Scott P Goulding<sup>1</sup>; Lia R Serrano<sup>1</sup>; Michael R Nelson<sup>1</sup>; Aman Makaju<sup>2</sup>; Jennifer G Abelin<sup>1</sup>; Terri A Addona<sup>1</sup>; <sup>1</sup>*Neon Therapeutics, Cambridge, MA*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*
- MP 593 **Intraspecific comparison of the venom peptidome of *Conus purpurascens*;** Meghan K. Grandal<sup>1, 2</sup>; Mickelene F. Hoggard<sup>1</sup>; Frank Mari<sup>1</sup>; <sup>1</sup>*National Institute of Standards and Technology, Charleston, SC*; <sup>2</sup>*Medical University of South Carolina, Charleston, SC*
- MP 598 **Enrichment of Zinc Finger Proteins by IMAC;** Stephanie Miller Lehman<sup>1</sup>; Josue Baeza<sup>1</sup>; Geoffrey P. Dann<sup>1</sup>; Benjamin A Garcia<sup>1</sup>; <sup>1</sup>*University of Pennsylvania, Philadelphia*
- MP 599 **A novel automated and highly selective phosphopeptide enrichment strategy for successful phosphopeptide identification and phosphosite localization;** Shuai Wu<sup>1</sup>; Kenneth Newton<sup>1</sup>; Linfeng Wu<sup>1</sup>; Jordy J. Hsiao<sup>1</sup>; Valery G. Voinov<sup>2, 3</sup>; Joseph S. Beckman<sup>2, 3</sup>; <sup>1</sup>*Agilent Technologies, Santa Clara, CA*; <sup>2</sup>*e-Msion Inc., Corvallis, OR*; <sup>3</sup>*Oregon State University, Corvallis, OR*
- MP 600 **A scalable phosphopeptide enrichment strategy for multiplexed quantitative phosphoproteomics;** Alison Erickson<sup>1</sup>; Brian Erickson<sup>1</sup>; Craig Braun<sup>1</sup>; Ryan Kunz<sup>1</sup>; <sup>1</sup>*IQ Proteomics LLC, Cambridge, MA*
- MP 601 **Large Scale EasyPep™ MS Sample Preparation for Phosphopeptide Enrichment Workflows;** Amarjeet Flora<sup>1</sup>; Ryan D. Bomgarden<sup>1</sup>; Sergei Snovidia<sup>1</sup>; Ashok Salunkhe<sup>1</sup>; John C. Rogers<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, Rockford, IL*





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- MP 610 **Dissection of flag leaf metabolic shifts and relationship with those occurring simultaneously in developing seed by application of non-targeted metabolomics;** Chaoyang Hu<sup>1</sup>; Jianxin Shi<sup>2</sup>; Yue Song<sup>3</sup>; Shan-an Chan<sup>4</sup>; <sup>1</sup>Ningbo University, Ningbo, China; <sup>2</sup>Shanghai Jiao Tong University, Shanghai, China; <sup>3</sup>Agilent Technologies, Shanghai, China; <sup>4</sup>Agilent Technologies, Taipei, Taiwan
- MP 620 **Proteomic analysis of translational control of gene expression under light treatment in Arabidopsis thaliana;** Yixiang Zhang<sup>1, 2</sup>; Xuhong Yu<sup>3</sup>; Scott D. Michaels<sup>3</sup>; Jonathan C. Trinidad<sup>1, 2</sup>; <sup>1</sup>Department of Chemistry, Indiana University, Bloomington, IN; <sup>2</sup>Laboratory for Biological Mass Spectrometry, Indiana University, Bloomington, IN; <sup>3</sup>Department of Biology, Indiana University, Bloomington, IN
- MP 625 **Utilization of Substructure Identification through MSn Analysis for Unknown Structure Determination Assisted with in silico Fragmentation Prediction;** Tim Stratton; Thermo Fisher Scientific, San Jose, CA
- MP 640 **Effect of amino acid supplementation on host cell protein profile for recombinant Pramlintide Concatemer production in E. coli;** Rohan Shah<sup>1</sup>; Saurabh Nagpal<sup>2</sup>; Anurag Rathore<sup>1</sup>; Jashwant Kumar<sup>1</sup>; <sup>1</sup>Indian Institute of Technology, delhi, India; <sup>2</sup>Agilent Technologies, Gurgaon, India
- MP 641 **Compiling a Method Toolbox to Improve Detection of Host Cell Proteins;** Martha Stapels<sup>1</sup>; Helena Awad<sup>1</sup>; Michelle Busch<sup>1</sup>; Joanne Cotton<sup>1</sup>; Fateme Tousi<sup>1</sup>; <sup>1</sup>Sanofi, Framingham, MA
- MP 642 **Monitoring of Non-human Glycan Motif in Biotherapeutics for Immunogenicity Prediction;** Unyong Kim<sup>1</sup>; Myung Jin Oh<sup>2, 3</sup>; Nari Seo<sup>2, 3</sup>; Hyun Joo An<sup>2, 3</sup>; <sup>1</sup>GLYCAN Co., Ltd., Seongnam, South Korea; <sup>2</sup>Asia-Pacific Glycomics Reference Site, Daejeon, South Korea; <sup>3</sup>Chungnam National University, Daejeon, South Korea
- MP 643 **Quantitative Analysis of Intact Monoclonal Antibodies from Mouse Serum using LC/MS and CE/MS Techniques;** David Wong<sup>1</sup>; Omar S. Barnaby<sup>2</sup>; Mei Han<sup>3</sup>; Yanan Yang<sup>1</sup>; Christopher A. James<sup>4</sup>; <sup>1</sup>Agilent Technologies, Inc., Santa Clara, CA; <sup>2</sup>Amgen, Inc., Thousand Oaks, CA; <sup>3</sup>Amgen Inc., South San Francisco, CA; <sup>4</sup>Amgen, Inc., Thousand Oaks, CA
- MP 644 **Spatially-resolved, 3D-printed Micro-sampling Coupled to Sensitive Nano-LC-MS to quantify the absolute levels of Heterogeneous Distribution of mAb/Targets in Tissues;** Ming Zhang<sup>1</sup>; Bo An<sup>1</sup>; Jun Qu<sup>1</sup>; <sup>1</sup>SUNY at Buffalo, Buffalo, NY
- MP 645 **Characterization of Commercial Vaccines by Charge Detection Mass Spectrometry;** Kevin Bond<sup>1</sup>; Che-Yen (Joe) Wang<sup>2</sup>; Martin F Jarrold<sup>1</sup>; <sup>1</sup>Indiana University Bloomington, Bloomington, IN; <sup>2</sup>Indiana University, Bloomington, IN
- MP 648 **A Generic Anti-Peptide Capture Coupled to LC/MS MRM for Low Level Pharmacokinetic Measurements of Therapeutic Proteins;** Bao-Jen Shyong<sup>1</sup>; Weixun Wang<sup>2</sup>; Huaibing He<sup>2</sup>; Bernard Choi<sup>2</sup>; Lucinda Hittle<sup>2</sup>; Kevin Bateman<sup>1</sup>; Daniel Spellman<sup>1</sup>; <sup>1</sup>Merck & Co., Inc., West Point, PA; <sup>2</sup>Merck & Co., Inc., Rahway, NJ
- MP 650 **Engineering the XS® Pichia Expression System to Reduce Host Cell Protein Impurities in Biopharmaceuticals Production;** Sylwia Jozwiak<sup>1</sup>; Katrien Claes<sup>2</sup>; Christoph Kiziak<sup>2</sup>; James Graham<sup>1</sup>; <sup>1</sup>Research and Development, Pharma&Biotech, Lonza Biologics plc, Slough, United Kingdom; <sup>2</sup>Research and Development Microbial, Pharma&Biotech, Lonza AG, Visp, Switzerland
- MP 651 **A High-Resolution Multi-Attribute Method for Product Characterization, Process Characterization, and Quality Control of Therapeutic Proteins;** Xiaoyan Guan<sup>1</sup>; Le Zhang<sup>1</sup>; Da Ren<sup>1</sup>; Tamer Eris<sup>1</sup>; <sup>1</sup>Amgen, Thousand Oaks, CA
- MP 655 **Tandem Quadrupole MS for the Quantification of Monoclonal Antibody Subunit Light Chains in Plasma;** Caitlin M Dunning<sup>1</sup>; Mary E Lame<sup>1</sup>; Yun W Alelyunas<sup>1</sup>; Mark D Wrona<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA
- MP 658 **Ultra-sensitive Quantification of Monoclonal antibodies and ADCs in Mouse Plasma using Trap-Elute MicroLC-MS/MS method;** Lei Xiong<sup>1</sup>; Ji Jiang<sup>1</sup>; Remco van Soest<sup>1</sup>; <sup>1</sup>Sciex, Redwood City, CA



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- MP 659 **Efficient data processing workflows for in-depth, MS-based glycoanalysis of biopharmaceuticals;** Aude Tartiere<sup>1</sup>; Albert Van Wyk<sup>2</sup>; Joe Shambaugh<sup>3</sup>; John McCarter<sup>3</sup>; Cassandra Wigmore<sup>4</sup>; Peter Haberl<sup>5</sup>; <sup>1</sup>*Genedata, Inc., San Francisco, CA*; <sup>2</sup>*Genedata Ltd, Cambridge, United Kingdom*; <sup>3</sup>*Genedata Inc, Lexington, MA, USA, Lexington, Massachusetts*; <sup>4</sup>*Genedata AG, Basel, Switzerland, Basel, Switzerland*; <sup>5</sup>*Genedata GmbH, Munich, Germany, Munich, Germany*
- MP 660 **Isotopically resolved Analysis of Protein Subunits using High Resolution Accurate Mass;** Sean Mccarthy<sup>1</sup>; Melanie Juba<sup>2</sup>; Zoe Zhang<sup>3</sup>; <sup>1</sup>*SCIEX, Framingham, MA*; <sup>2</sup>*Sciex, Framingham, MA*; <sup>3</sup>*Sciex, Redwood City, CA*
- MP 669 **Automated Chemical Footprinting Enables Monitoring of Conformational Change of Protein Therapeutics;** Sonya Entova<sup>1</sup>; Nina Chen<sup>1</sup>; Mohammed Sahar<sup>1</sup>; Alla Polozova<sup>1</sup>; Hao Zhang<sup>1</sup>; <sup>1</sup>*Amgen Inc., Cambridge, MA*
- MP 670 **Time-resolved Deconvolution for Automated, In-depth Characterization of an IgG-type Monoclonal Antibody by Intact Mass Analysis;** Peter Haberl<sup>1</sup>; John McCarter<sup>2</sup>; Aude Tartiere<sup>3</sup>; Albert Van Wyk<sup>4</sup>; Cassandra Wigmore<sup>5</sup>; Joe Shambaugh<sup>2</sup>; <sup>1</sup>*Genedata GmbH, Munich, Germany*; <sup>2</sup>*Genedata, Inc., Lexington, MA*; <sup>3</sup>*Genedata, Inc., San Francisco, CA*; <sup>4</sup>*Genedata Ltd, Cambridge, United Kingdom*; <sup>5</sup>*Genedata AG, Basel, Switzerland*
- MP 672 **A workflow-driven platform solution for MAM-based critical quality attribute monitoring of biotherapeutics in process development and QC;** Nilini Ranbaduge<sup>1</sup>; Henry Shion<sup>1</sup>; Ying Qing Yu<sup>1</sup>; Min Du<sup>1</sup>; Weibin Chen<sup>1</sup>; <sup>1</sup>*Waters Corporation, Milford, MA*
- MP 674 **High-Throughput Analysis of Antibody Charge Heterogeneity by Native Microfluidic Capillary Electrophoresis- Mass Spectrometry;** Hongxia (jessica) Wang<sup>1</sup>; Haibo Qiu<sup>1</sup>; Jikang Wu<sup>1</sup>; Thomas Daly<sup>1</sup>; Ning Li<sup>1</sup>; <sup>1</sup>*Regeneron Pharmaceuticals Inc., Tarrytown, NY*
- MP 676 **Improved middle-down characterization of antibodies using multiple ion activation techniques and Proton Transfer Reaction on a modified Orbitrap mass spectrometer;** Romain Huguet<sup>1</sup>; Kristina Srzentic<sup>2</sup>; John E. P. Syka<sup>1</sup>; Christopher Mullen<sup>1</sup>; Joshua A Silveira<sup>1</sup>; Jennifer Sutton<sup>1</sup>; Luca Fornelli<sup>3</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*Thermo Fisher Scientific, Cambridge, MA*; <sup>3</sup>*University of Oklahoma, Health and Science Center, Norman, Afghanistan*
- MP 680 **The Investigation of High Intensity Interval Training on Left Ventricular Fibrosis in Cardiac Patients by Proteomics;** Meng-chu Liu<sup>1</sup>; Pang-Hung Hsu<sup>1</sup>; Chih-Chin Hsu<sup>2</sup>; <sup>1</sup>*Department of Bioscience and Biotechnology, National Taiwan Ocean University, Keelung City, Taiwan*; <sup>2</sup>*Department of Physical Medicine and Rehabilitation, Keelung Chang Gung Memorial Hospital, Keelung City, Taiwan*
- MP 683 **Identifying Quantitative Protein Changes in the Iris of Glaucoma Patients Using Label Free Proteomics;** Craig P Dufresne<sup>1</sup>; Richard D Semba<sup>2</sup>; Pingbo Zhang<sup>2</sup>; Min Zhu<sup>2</sup>; Jiang Qian<sup>3</sup>; Tianshun Gao<sup>2</sup>; Ibrahim AlJadaan<sup>4</sup>; Sami AlShahwan<sup>4</sup>; Ohood Owaidha<sup>4</sup>; Randy Craven<sup>2</sup>; Deepak Edward<sup>2, 4</sup>; Alka Mahale<sup>4</sup>; <sup>1</sup>*Thermo Fisher Scientific, West Palm Beach, FL*; <sup>2</sup>*Johns Hopkins University, Baltimore, MD*; <sup>3</sup>*National Institute on Aging, National Institutes of Health, Baltimore, MD*; <sup>4</sup>*King Khaled Eye Specialist Hospital, Riyadh, Saudi Arabia*
- MP 685 **Application of plasma proteomics in Alzheimer's Disease;** Mostafa J Khan<sup>1</sup>; Renã A.S. Robinson<sup>1</sup>; <sup>1</sup>*Vanderbilt University, Nashville, TN*
- MP 689 **Proteomic analysis of Dpy19l2-deficient human globozoospermia reveals multiple molecular defects;** Xuejiang Guo<sup>1</sup>; Yueshuai Guo<sup>1</sup>; Daozhen Chen<sup>2</sup>; Xiaoyu Yang<sup>1</sup>; <sup>1</sup>*Nanjing Medical University, Nanjing, China*; <sup>2</sup>*Wuxi Maternal and Child Health Care Hospital Affiliated to Nanjing Medical University, Wuxi, China*
- MP 703 **Method development for the identification of proteins in fingertip smears by using MALDI-MS;** Cristina Russo<sup>1</sup>; Laura Cole<sup>1</sup>; Lynda Wyld<sup>2</sup>; Simona Francese<sup>1</sup>; <sup>1</sup>*Sheffield Hallam University, Sheffield, United Kingdom*; <sup>2</sup>*The University of Sheffield, Sheffield, United Kingdom*



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- MP 708 **Identifying breast cancer vulnerabilities by mapping interactome dysregulations in primary tumor samples;** Johannes Kreuzer<sup>1</sup>; Robert Morris<sup>1</sup>; Ridwan Ahmad<sup>1</sup>; Cyril H. Benes<sup>1</sup>; Dennis C. Sgroi<sup>1</sup>; Wilhelm Haas<sup>1</sup>; <sup>1</sup>*Massachusetts General Hospital and Harvard Medical School, Charlestown, MA*
- MP 710 **Evaluation of different sample preparation workflows for reproducible, quantitative, and in-depth analysis of urine proteomics;** Hua Ding<sup>1</sup>; Hossein Fazelinia<sup>1</sup>; Lynn A. Spruce<sup>1</sup>; Dana A. Weiss<sup>1</sup>; Stephen A. Zderic<sup>1</sup>; Steven H. Seeholzer<sup>1</sup>; <sup>1</sup>*Children's Hospital of Philadelphia, Philadelphia, PA*
- MP 713 **MS-based deep proteome profiling of AD related mouse model defective in RNA splicing;** Mingming Niu<sup>1</sup>; Ping-Chung Chen<sup>2</sup>; Yun Jiao<sup>2</sup>; Hong Wang<sup>2</sup>; Junmin Peng<sup>2</sup>; <sup>1</sup>*St Jude Children's Research Hospital, Memphis, TN*; <sup>2</sup>*St Jude Children's Research Hospital, Memphis, TN*
- MP 715 **Comparison of quantitative LC/MS/MS plant protein assay design and impact on precision of results;** Kristi Harkins<sup>1</sup>; Danielle Baker<sup>1</sup>; Michaela Owens<sup>1</sup>; <sup>1</sup>*DowDuPont, Johnston, IA*
- MP 718 **Systematic Investigation of Protein Dynamics to Unveil Their Degradation Pathways in Human Cells;** Ming Tong<sup>1</sup>; Ronghu Wu<sup>1</sup>; <sup>1</sup>*Georgia Institute of Technology, Atlanta, GA*
- MP 728 **Protein Assisted Digestion Improves Sensitivity of Immunocapture-MRM Method to Quantify Stool Biomarker of Colorectal Cancer;** Rebecca Bearden<sup>1</sup>; Baochuan Guo<sup>1</sup>; <sup>1</sup>*Cleveland State University, Cleveland, OH*
- MP 730 **Characterization of the Ubiquitination Signaling on Hypoxia-Inducible Factor with Quantitative Chemical Proteomics Analysis;** Yunan Li<sup>1</sup>; Ang Luo<sup>1</sup>; Luke Erber<sup>1</sup>; Yue Chen<sup>1</sup>; <sup>1</sup>*University of Minnesota at Twin Cities, Minneapolis, MN*
- MP 732 **Evaluation of the Accuracy of Synchronous Precursor Selection (SPS) in Public Datasets;** Conor Jenkins<sup>1,2</sup>; Aimee Rinas<sup>3</sup>; Benjamin Orsburn<sup>1</sup>; <sup>1</sup>*Think20 Labs, Columbia, MD*; <sup>2</sup>*Hood College Bioinformatics Program, Frederick, MD*; <sup>3</sup>*AIT BioSciences, Indianapolis, IN*
- MP 733 **Applications of Mass Spectrometry Targeted Assays for Quantitative Analysis of Cancer Signaling Proteins;** Penny Jensen<sup>1</sup>; Bhavin Patel<sup>1</sup>; Leigh A Foster<sup>1</sup>; Aaron S. Gajadhar<sup>2</sup>; Sebastien Gallien<sup>3</sup>; Jonathan R Krieger<sup>4</sup>; Jiefei Tong<sup>5</sup>; Michael F. Moran<sup>4</sup>; Rosa Viner<sup>2</sup>; Andreas Huhmer<sup>2</sup>; Kay Opperman<sup>1</sup>; John C Rogers<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, Rockford, IL*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>3</sup>*Thermo Fisher Scientific, Precision Medicine Science Center, Cambridge, MA*; <sup>4</sup>*SPARC BioCentre, Hospital for Sick Children, Toronto, Ontario*; <sup>5</sup>*Program in Cell Biology, The Hospital for Sick Children, Toronto, Ontario*
- MP 749 **A Novel Proteomic Method Defines Extracellular Matrix Proteins and Their Post-Translational Modifications from Formalin-Fixed, Paraffin-Embedded Specimens of Heart Valve Disease;** Cassandra L Clift<sup>1</sup>; Susana Comte-Walters<sup>1</sup>; Lauren E Ball<sup>1</sup>; David Bichell<sup>2</sup>; Yan Ru Su<sup>3</sup>; Anand Mehta<sup>1</sup>; Richard R Drake<sup>1</sup>; Peggi M. Angel<sup>1</sup>; <sup>1</sup>*Department of Cell and Molecular Pharmacology and Experimental Therapeutics, Medical University of South Carolina, Charleston, SC*; <sup>2</sup>*Division of Pediatric Cardiac Surgery, Vanderbilt University Medical Center, Nashville, TN*; <sup>3</sup>*Department of Cardiovascular Medicine, Vanderbilt University Medical Center, Nashville, TN*
- MP 751 **Proteomic analysis of extracellular matrix dynamics during mouse forelimb development;** Kathryn R Jacobson<sup>1</sup>; Sarah L Lipp<sup>1</sup>; Alex R. Ocken<sup>1</sup>; Tamara L. Kinzer-Ursem<sup>1</sup>; Sarah Calve<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*
- MP 752 **Extensive Intratumor Proteogenomic Heterogeneity Revealed by Multiregion Sampling in a High-Grade Serous Ovarian Tumor Specimen;** Thomas P. Conrads<sup>1,2</sup>; Allison L. Hunt<sup>1</sup>; Guisong Wang<sup>2</sup>; Julie Oliver<sup>2</sup>; Dave Mitchell<sup>2</sup>; Glenn Gist<sup>2</sup>; Brian Hood<sup>2</sup>; Ming Zhou<sup>1</sup>; Brian Blanton<sup>2</sup>; Kelly Conrads<sup>2</sup>; Chad Hamilton<sup>2</sup>; Kathleen Darcy<sup>2</sup>; Craig Shriver<sup>3</sup>; Yovanni Casablanca<sup>2</sup>; George Larry Maxwell<sup>2</sup>; Nicholas W. Bateman<sup>2</sup>; <sup>1</sup>*Inova Schar Cancer Institute, Annandale, VA*; <sup>2</sup>*Gynecologic Cancer Center of Excellence, Annandale, VA*; <sup>3</sup>*John P. Murtha Cancer Center, Bethesda, MD*
- MP 756 **Identification and Validation of Synapse-Loss Regulating Phosphorylation Events in Schizophrenia;** Megan Garver<sup>1</sup>; Ying Ding<sup>2</sup>; Robert Sweet<sup>1</sup>; Nathan A Yates<sup>3</sup>; Matthew L MacDonald<sup>1</sup>; <sup>1</sup>*UPMC, Pittsburgh,*



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- MP 761 *PA*; <sup>2</sup>Department of Biostatistics, University of Pittsburgh, Pittsburgh, Pennsylvania; <sup>3</sup>BioMS Center, University of Pittsburgh, Pittsburgh, Pennsylvania  
**A Label-free Quantification Approach to Identify Differentially Expressed Proteins between Wild Type and Transgenic Alzheimer Rat Brains;** Pritha Bagchi<sup>1</sup>; Eric B. Dammer<sup>1</sup>; Geng M. Wang<sup>1</sup>; Robert M. Cohen<sup>2</sup>; Nicholas T. Seyfried<sup>1,3</sup>; <sup>1</sup>Emory Integrated Proteomics Core, Emory University, Atlanta, Georgia; <sup>2</sup>Department of Psychiatry and Behavioral Sciences, Emory University, Atlanta, Georgia; <sup>3</sup>Department of Biochemistry, Emory University, Atlanta, Georgia
- MP 776 **Extending the mass range for Native Top-Down Mass Spectrometry by UVPD;** Jean-Francois Greisch<sup>1,2</sup>; Sem Tamara<sup>1,2</sup>; Albert J.R. Heck<sup>1,2</sup>; <sup>1</sup>Biomolecular Mass Spectrometry and Proteomics, Bijvoet Center for Biomolecular Research and Utrecht Institute of Pharmaceutical Sciences, Utrecht University, Utrecht, Netherlands; <sup>2</sup>Netherlands Proteomics Center, Utrecht, Netherlands
- MP 783 **Profiling Combinatorial Posttranslational Modifications in Seminal Plasma from Dairy Bulls via Sheathless Capillary Zone Electrophoresis – Top-Down Mass Spectrometry;** Fabio P. Gomes<sup>1</sup>; Jolene K. Diedrich<sup>1</sup>; Anthony J. Saviola<sup>1</sup>; Abdullah Kaya<sup>2</sup>; Erdogan Memili<sup>3</sup>; Arlindo A. Moura<sup>4</sup>; John R. Yates, III<sup>1</sup>; <sup>1</sup>The Scripps Research Institute, La Jolla, CA; <sup>2</sup>Selcuk University, Selçuklu, Turkey; <sup>3</sup>The Mississippi State University, Starkville, MS; <sup>4</sup>The Federal University of Ceara, Fortaleza, Brazil
- TP 002 **Analysis of therapeutic monoclonal antibodies using volatile pH gradient cation exchange chromatography directly coupled to native mass spectrometry;** Julia Baek<sup>1</sup>; Rosa Viner<sup>2</sup>; Terry Zhang<sup>2</sup>; James Ngai<sup>3</sup>; Eugen Damoc<sup>4</sup>; Shanhua Lin<sup>5</sup>; <sup>1</sup>Thermo Fisher Scientific, Sunnyvale, California; <sup>2</sup>Thermo Fisher Scientific, San Jose, California; <sup>3</sup>Thermo Fisher Scientific, Sunnyvale; <sup>4</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>5</sup>Thermo Fisher Scientific, Sunnyvale, CA
- TP 009 **Application of wildcard search approach in sequence variant analysis;** Yutian Gan; Genentech, Inc., South San Francisco, CA
- TP 015 **Automated comprehensive characterization and quantification of low-abundance sequence variants in a standard monoclonal antibody;** Joe Shambaugh<sup>1</sup>; Aude Tartiere<sup>2</sup>; Albert Van Wyk<sup>3</sup>; John McCarter<sup>4</sup>; Cassandra Wigmore<sup>5</sup>; Peter Haberl<sup>6</sup>; <sup>1</sup>Genedata Inc, Lexington, MA; <sup>2</sup>Genedata, Inc., San Francisco, CA; <sup>3</sup>Genedata Ltd, Cambridge, United Kingdom; <sup>4</sup>Genedata, Inc., Lexington, MA; <sup>5</sup>Genedata AG, Basel, Switzerland; <sup>6</sup>Genedata GmbH, Munich, Germany
- TP 018 **Native Top-Down Analysis of Intact Antibodies using Multiple Dissociation Techniques on a Tribrid Quadrupole Orbitrap Linear Ion Trap Mass Spectrometer;** Eugen Damoc<sup>1</sup>; Kristina Srzenti<sup>2</sup>; Romain Huguet<sup>3</sup>; Graeme Mcalister<sup>3</sup>; Christopher Mullen<sup>3</sup>; Philip M Remes<sup>3</sup>; Jesse D Canterbury<sup>3</sup>; Mike Senko<sup>3</sup>; Vlad Zabrouskov<sup>3</sup>; <sup>1</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>2</sup>Thermo Fisher Scientific, Cambridge, Massachusetts; <sup>3</sup>Thermo Fisher Scientific, San Jose, California
- TP 019 **Process Monitoring of Monoclonal Antibodies at Intact and Subunits Levels using a Single Quadrupole LC/MS for Quality Control;** Linfeng Wu<sup>1</sup>; Lisa Zang<sup>1</sup>; Guannan Li<sup>1</sup>; Tom Chen<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA
- TP 039 **Proteomic and lipidomic analysis reveals altered fatty acid metabolism in the liver of the symptomatic Niemann-Pick, type C1 mouse model;** Melissa R Pergande<sup>1</sup>; Jonathon Hanek<sup>1</sup>; Estefanía Zárate<sup>1</sup>; Sheher Banu Mohsin<sup>2</sup>; Carol Haney-Ball<sup>3</sup>; Stephanie M Cologna<sup>1</sup>; <sup>1</sup>University of Illinois at Chicago, Chicago, IL; <sup>2</sup>Agilent Technologies, Wood Dale, IL; <sup>3</sup>Agilent Technologies, Cary, NC
- TP 040 **Epitope Structures of Aptamer Complexes of the Multi-domain Protein C-Met Revealed by Proteolytic Affinity- Mass Spectrometry;** Michael Przybylski<sup>1</sup>; Loredana Lupu<sup>2</sup>; Pascal Wiegand<sup>2</sup>; Nico Hüttmann<sup>2</sup>; Stephan Rawer<sup>2</sup>; Wolfgang Kleinekofort<sup>2,3</sup>; Irina Shchugoreva<sup>4</sup>; Anna S. Kichkailo<sup>5</sup>; Felix N. Tomilin<sup>4</sup>; Alexander Lazarev<sup>6</sup>; Maxim V. Berezovski<sup>7</sup>; <sup>1</sup>Steinbeis Centre Biopolymer Analysis and Biomedical Mass Spectrometry, Ruesselsheim, Germany; <sup>2</sup>Steinbeis Centre Biopolymer Analysis and Biomedical Mass Spectrometry, Ruesselsheim, Germany; <sup>3</sup>Rhein Main University, Rüsselsheim, Germany; <sup>4</sup>Kirensky



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- Institute of Physics, Russian Academy of Sciences, Krasnoyarsk, Russia; <sup>5</sup>Krasnoyarsk State Medical University, Krasnoyarsk, Russia; <sup>6</sup>Pressure Biosciences Inc., South Easton, MA; <sup>7</sup>University of Ottawa, Dept. Chemistry, Ottawa, Quebec*
- TP 043 **Targeted Metabolomics Profile Sow Milk Components by LC-MS/MS;** Shen Allison<sup>1</sup>; Qisheng Zhong<sup>2</sup>; <sup>1</sup>Shimadzu Global COE, Shimadzu (China) Co., Ltd., China, Guangzhou, China; <sup>2</sup>Shimadzu Global COE, Shimadzu (China) Co., Ltd., China, Guangzhou, China
- TP 045 **Identification of novel serum protein biomarkers for ALS diagnosis and progression;** Szymon Filip<sup>1</sup>; Tori Sosnowski<sup>1</sup>; Halil Idrisoglu<sup>2</sup>; Hande Ozdinler<sup>3, 4</sup>; Young Ah Goo<sup>1</sup>; <sup>1</sup>Proteomics Center of Excellence, Northwestern University, Chicago, ILLINOIS; <sup>2</sup>Istanbul University, Istanbul, Turkey; <sup>3</sup>Department of Neurology, Northwestern University, Feinberg School of Medicine, Chicago, ILLINOIS; <sup>4</sup>Les Turner ALS Center at Northwestern University, Chicago, ILLINOIS
- TP 066 **Protein identification - the translational research study of HBx genes related to hepatocellular carcinoma;** Ming-Hui Yang<sup>1</sup>; Yi-Ming Arthur Chen<sup>2</sup>; Yi-Chia Lee<sup>3</sup>; Yu-Chang Tyan<sup>3</sup>; <sup>1</sup>National Health Research Institutes, Zhunan, Taiwan; <sup>2</sup>Taipei Medical University, Taipei, Taiwan; <sup>3</sup>Kaohsiung Medical University, Kaohsiung, Taiwan
- TP 073 **Quantification of Soluble MERTK in Serum Using Affinity Enrichment-Liquid Chromatography Mass Spectrometry;** Yongxin Zhu<sup>1</sup>; Petia Shipkova<sup>2</sup>; Thomas Spires<sup>2</sup>; Karen Augustine<sup>2</sup>; Timothy Olah<sup>2</sup>; <sup>1</sup>Bristol-Myers Squibb Company, Princeton, NJ; <sup>2</sup>Bristol-Myers Squibb Co., Princeton, NJ
- TP 078 **Development of an automated sample preparation platform for cPILOT;** Albert Arul<sup>1</sup>; Renã A.S. Robinson<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN
- TP 080 **Measurement of cyclooxygenase inhibition and selectivity in human whole blood assay using LC-MS/MS;** Yifan Shi<sup>1</sup>; Heather Murrey<sup>1</sup>; Kay Ahn<sup>1</sup>; Naidong Weng<sup>1</sup>; Shefali Patel<sup>1</sup>; <sup>1</sup>Janssen, Spring House, PA
- TP 089 **LC-MS/MS Analysis of Arachidonic Acid as a Biomarker in Human Plasma for Clinical Studies;** Tian-Sheng Lu<sup>1</sup>; Elise Snider<sup>1</sup>; Nicole Greer<sup>1</sup>; Joshua Froning<sup>1</sup>; Yong-Xi Li<sup>1</sup>; <sup>1</sup>Medpace Bioanalytical Laboratories, Cincinnati, OH
- TP 090 **Developing protein biomarker MRM methods as an alternative indicator of prohibited substance abuse in Equine athletes;** Sophie Bromilow<sup>1</sup>; Heather Knych<sup>1</sup>; Ben Moeller<sup>1</sup>; Rick Arthur<sup>1</sup>; Claudia P.B. Martins<sup>2</sup>; David Horohov<sup>3</sup>; Scott Stanley<sup>3</sup>; <sup>1</sup>K.L. Maddy Equine Analytical Chemistry Laboratory, Davis, CA; <sup>2</sup>ThermoFisher, San Jose, CA; <sup>3</sup>Gluck Equine Research Centre, Lexington, Kentucky
- TP 093 **Dried blood spots from frozen whole blood provide an option to analyze Parkinson's disease cohorts for activity of lysosomal enzymes;** Pavlina Wolf<sup>1</sup>; Roy Alcalay<sup>2</sup>; Karolina Helesicova<sup>1</sup>; Ruby Chiang<sup>1</sup>; Emma-Jane Turton<sup>1</sup>; Michael Pauciulo<sup>3</sup>; William Nichols<sup>3</sup>; Wendy Chung<sup>4</sup>; Pablo Sardi<sup>1</sup>; Kate Zhang<sup>1</sup>; Petra Oliva<sup>1</sup>; <sup>1</sup>Sanofi, Framingham, MA; <sup>2</sup>Columbia University Medical Center, Neurological Institute, New York, NY; <sup>3</sup>Division of Human Genetics, Cincinnati Children's Hospital Medical Center and the Department of Pediatrics, University of Cincinnati College of Medicine, Cincinnati, Ohio; <sup>4</sup>Department of Pediatrics and Medicine, Columbia University Medical Center, New York, NY
- TP 095 **Multiplexed quantification of sepsis prognosis candidate biomarkers spanning a wide dynamic range of plasma concentrations (ng/ml to mg/ml);** Christelle Dubois<sup>1</sup>; Didier Payen<sup>2</sup>; Stéphanie Simon<sup>1</sup>; François Fenaille<sup>1</sup>; Christophe Junot<sup>1</sup>; Nathalie Morel<sup>1</sup>; François Becher<sup>1</sup>; <sup>1</sup>CEA Saclay, DRF, Institut Joliot, Service de Pharmacologie et d'Immunoanalyse- CEA-INRA UMR 0496, Laboratoire d'Etude du Métabolisme des Médicaments, Gif-sur-Yvette, France; <sup>2</sup>Department of Anesthesiology and Critical Care, Lariboisière Hospital, University of Paris Denis Diderot 7, Paris, France
- TP 096 **Metaproteomics of the human intestinal microbiota in physiological and pathological conditions;** celine Henry<sup>1</sup>; Ariane Bassignani<sup>2, 3</sup>; Olivier Langella<sup>4</sup>; Véronique Monnet<sup>2</sup>; Catherine Juste<sup>2</sup>; the ProteoCardis Consortium<sup>1, 2, 4, 5, 6, 7</sup>; <sup>1</sup>PAPPSO, Micalis Institute, INRA, AgroParisTech, Université Paris-



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- TP 102 **Transition Ratios for the Product-Ion-Poor: Activation Energy Modulation in the Absence of Distinct Neutral Losses;** Brian Rappold; *LabCorp, Raleigh, NC*
- TP 115 **Revealing Proteomic Subgroups with Clinical Classification and Prognostic Prediction in Pancreatic Ductal Adenocarcinoma using MRM-MS;** Minsoo Son<sup>1</sup>; Yoseop Kim<sup>1</sup>; Jinyoung Jang<sup>2</sup>; Youngsoo Kim<sup>1</sup>; <sup>1</sup>*Department of Biomedical Engineering, Seoul National University College of Medicine, Jongro-gu, South Korea; <sup>2</sup>Department of surgery, Seoul National University College of Medicine, Jongro-gu, South Korea*
- TP 118 **Bioanalytical method for quantification of polymyxin B1, polymyxin B2, polymyxin B3 and isoleucine-polymyxin B1 in human plasma;** Peiling Hou<sup>1</sup>; Shu Qing Chan<sup>\*2</sup>; Jie Xing<sup>3</sup>; <sup>1</sup>*Application Development & Support Centre, Shimadzu (Asia Pacific) Pte Ltd., 79 Science Park Drive #02-01/08, Singapore; <sup>2</sup>School of Chemical and Life Sciences, Singapore Polytechnic, 500 Dover Road, Singapore; <sup>3</sup>Application Development & Support Centre, Shimadzu (Asia Pacific) Pte Ltd, 79 Science Park Drive #02-01/08, Singapore*
- TP 134 **Detection of Anthrax toxins in terminal organ tissues by mass spectrometry;** Maribel Gallegos Candela<sup>1</sup>; Anne E Boyer<sup>1</sup>; Adrian R. Woolfitt<sup>1</sup>; Renato C. Lins<sup>2</sup>; Maria I. Solano<sup>1</sup>; John R. Barr<sup>1</sup>; <sup>1</sup>*Center for Disease Control, Atlanta, GA 30341; <sup>2</sup>Battelle Integrated Science Solutions, Atlanta, GA 30329*
- TP 140 **Is NAP treatment a solution for neuroprotection in ADNP mutation syndrome?;** Ming-Hui Yang<sup>1</sup>; Yi-Chia Lee<sup>2</sup>; Hsin-Yi Wu<sup>3</sup>; Ko-Chin Chen<sup>4</sup>; Yi-Ming Arthur Chen<sup>5</sup>; Yu-Chang Tyan<sup>2</sup>; <sup>1</sup>*National Health Research Institutes, Zhunan, Taiwan; <sup>2</sup>Kaohsiung Medical University, Kaohsiung, Taiwan; <sup>3</sup>National Taiwan University, Taipei, Taiwan; <sup>4</sup>Changhua Christian Hospital, Changhua, Taiwan; <sup>5</sup>Taipei Medical University, Taipei, Taiwan*
- TP 147 **Inductively Coupled Plasma-Mass Spectrometry Characterization of Asphaltene Metals Pre- and Post-Cleanup for Enhanced Nuclear Magnetic Resonance Spectroscopy Results;** Annie E. Arvidson<sup>1</sup>; Ian G. M. Anthony<sup>1</sup>; Michael T. Spiegel<sup>1</sup>; Shubhneet Warar<sup>1</sup>; Patrick J. Farmer<sup>1</sup>; Touradj Solouki<sup>1</sup>; <sup>1</sup>*Baylor University, Waco, TX*
- TP 150 **CID fragmentation studies of asphaltenes at different precipitation times using Magnetic Resonance Mass Spectrometry (MRMS);** Matthias Witt<sup>1</sup>; Michael L. Easterling<sup>2</sup>; Estrella Rogel<sup>3</sup>; <sup>1</sup>*Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup>Bruker Daltonics Inc., Billerica, MA; <sup>3</sup>Chevron, Richmond, CA*
- TP 152 **Evaluation of Time Effects on Precipitated Asphaltene Characteristics using APPI and LDI coupled to Magnetic Resonance Mass Spectrometry (MRMS);** Estrella Rogel<sup>1</sup>; Matthias Witt<sup>2</sup>; Michael Moir<sup>1</sup>; <sup>1</sup>*Chevron, Richmond, CA; <sup>2</sup>Bruker Daltonik GmbH, Bremen, Germany*
- TP 155 **(+/-) ESI FT MS Analysis of Crude Oils from the Volga-Ural region;** Vlad Lobodin<sup>1</sup>; Dmitrii Mazur<sup>2</sup>; Roman Borisov<sup>3</sup>; <sup>1</sup>*MAXIKAT, INC, Tallahassee, FL; <sup>2</sup>The Department of Chemistry, Moscow State University, Moscow, Russia; <sup>3</sup>A.V. Topchiev Institute of Petrochemical Synthesis, Moscow, Russia*
- TP 161 **Analysis of drinking water for determination of Volatile Organic Components (VOC's) using Dynamic Headspace Gas Chromatography Mass Spectrometry;** Sanket Anand Chiplunkar<sup>1</sup>; Dheeraj Handique<sup>1</sup>; Prashant Hase<sup>1</sup>; Durvesh Sawant<sup>1</sup>; Nitish Suryawanshi<sup>1</sup>; Aseem Wagle<sup>1</sup>; Pratap Rasam<sup>1</sup>; Jitendra Kelkar<sup>1</sup>; Ajit Datar<sup>1</sup>; Satyendra Thakur<sup>2</sup>; Sunil Singh<sup>2</sup>; <sup>1</sup>*Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India; <sup>2</sup>Shimadzu Analytical (India) Pvt. Ltd., New Delhi, India*



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- TP 166 **Improved non-target screening based identification of organic micropollutants in water samples;** Andrea Mizzi Brunner<sup>1</sup>; Seema Sharma<sup>2</sup>; Christian Panse<sup>3</sup>; Romain Huguet<sup>2</sup>; Dennis Vughs<sup>1</sup>; Vlad Zabrouskov<sup>2</sup>; Annemieke Kolkman<sup>1</sup>; <sup>1</sup>*KWR Watercycle Research Institute, Nieuwegein, Netherlands*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, Ca, 95134*; <sup>3</sup>*Functional Genomics Center Zurich, Zurich, Switzerland*
- TP 188 **Determination of 8 nitrosamines in water by liquid chromatography coupled to tandem mass spectrometry;** Wei Du<sup>1</sup>; Xiaorong Ran<sup>1</sup>; <sup>1</sup>*Agilent Technologies(China) Co. Ltd., Beijing, China*
- TP 191 **Methods for Metaproteomic Analysis of the Ocean;** Matthew McIlvin<sup>1</sup>; Mak Saito<sup>2</sup>; <sup>1</sup>*Woods Hole Oceanographic Inst., Woods Hole, MA*; <sup>2</sup>*Woods Hole Oceanographic Institution, Woods Hole*
- TP 194 **Quantification of Azithromycin in sheep tissue samples using LCMSMS;** Chander Mani<sup>1</sup>; T.s. Lohith<sup>2</sup>; Saikat Banerjee<sup>1</sup>; Samir Vyas<sup>1</sup>; S.m. Byregowda<sup>2</sup>; K. Sripad<sup>2</sup>; <sup>1</sup>*Agilent Technologies, Gurgaon, India*; <sup>2</sup>*Institute of Animal Health and Veterinary Biologicals, Bengaluru, India*
- TP 195 **Developing methods to assess the environmental impact of pesticides and pharmaceuticals on aquatic fauna using targeted and untargeted HRAM Q-TOF;** Christopher Titman<sup>1</sup>; Thomas H Miller<sup>2</sup>; Keng Tiong Ng<sup>2</sup>; Nicholas R Bury<sup>3,4</sup>; Leon P Barron<sup>2</sup>; Alan Barnes<sup>5</sup>; Neil Loftus<sup>5</sup>; <sup>1</sup>*Shimadzu UK Limited, Milton Keynes, United Kingdom*; <sup>2</sup>*Department of Analytical, Environmental & Forensic Sciences, School of Population Health & Environmental Sciences, Faculty of Life Sciences and Medicine, King's College London, United Kingdom*; <sup>3</sup>*School of Science, Technology and Engineering, University of Suffolk, James Hehir Building, University Avenue, Ipswich, United Kingdom*; <sup>4</sup>*Division of Diabetes and Nutritional Sciences, Faculty of Life Sciences and Medicine, King's College London, Franklin Wilkins Building, United Kingdom*; <sup>5</sup>*Shimadzu Corporation, Manchester, United Kingdom*
- TP 197 **ESS-MAT: A new approach for simultaneous analysis of organophosphate pesticides and their degradation products on agricultural products;** noam Kirshenbaum<sup>1</sup>; Tamara Polubesova<sup>1</sup>; Benny Chefetz<sup>1</sup>; <sup>1</sup>*Department of Soil and Water Sciences The Robert H. Smith Faculty of Agriculture, Food and Environment The Hebrew University of Jerusalem, Rehovot, Israel*
- TP 202 **Fast Creatinine Determination in Wastewater by Liquid Chromatography-Mass Spectrometry;** Lisa Wanders<sup>1</sup>; Matthew Obusek<sup>1</sup>; <sup>1</sup>*Thomson Instrument Co, Oceanside, CA*
- TP 215 **Determination of Polar Pesticides in Grapes Using a Compact Ion Chromatography System Coupled with Tandem Mass Spectrometry;** Beibei Huang<sup>1</sup>; Jeffrey Rohrer<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, Sunnyvale*
- TP 216 **Highly sensitive direct analysis of glyphosate, glufosinate and AMPA in the beverages by LC-MS / MS;** Manami Kobayashi<sup>1</sup>; Miho Kawashima<sup>2</sup>; Yusuke Inohana<sup>2</sup>; Nozomi Maeshima<sup>1</sup>; Junichi Masuda<sup>1</sup>; Yoshihiro Hayakawa<sup>2</sup>; <sup>1</sup>*Shimadzu Corporation, Hadano, Japan*; <sup>2</sup>*Shimadzu Corporation, Kyoto, Japan*
- TP 227 **Simultaneous determination of 130 veterinary drug in pork using ultra performance liquid chromatograph-tandem mass spectrometry;** Zhao Liu; *Shimadzu (China) Co.,Ltd., Shanghai, China*
- TP 229 **Separation and quantification of N-acetyl-cysteine and glutathione by isotopic iodoacetamide modification and HILIC coupled with tandem mass spectrometry;** Shih-shin Liang; *Kaohsiung Medical University, Kaohsiung, Taiwan*
- TP 230 **Rapid screening and quantitative analysis of pesticides in vegetables by liquid chromatography tandem quadrupole time of flight mass spectrometry;** Biao Ren; *Shimadzu(China)Co.,LTD.Beijing Branch, Beijing, China*
- TP 231 **Simultaneous determination of tebufenozide and indoxacarb in animal products using liquid-liquid extraction method coupled with liquid chromatography-tandem mass spectrometry;** Kyung-Hee Yoo<sup>1</sup>; Da-hee Park<sup>1</sup>; Seong-Kwan Kim<sup>1</sup>; Ho-Chul Shin<sup>1</sup>; <sup>1</sup>*Konkuk university, Seoul, South Korea*
- TP 239 **Targeted screening and quantitation of pesticide residues in green tea using a Quadrupole Time-of-Flight Mass Spectrometer;** Toshiya Matsubara<sup>1</sup>; Huan Lin<sup>1</sup>; Natsuyo Asano<sup>1</sup>; Mikie Shima<sup>2</sup>; <sup>1</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>2</sup>*AiSTI Science Co., Ltd., Wakayama, Japan*



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- TP 240 **Simultaneous determination of pesticide residues in vegetable extract by liquid chromatograph tandem mass spectrometry for high recovery rate;** Nozomi Maeshima<sup>1</sup>; Manami Kobayashi<sup>1</sup>; Masuda Junichi<sup>1</sup>; <sup>1</sup>*Shimadzu Corporation, Hadano, Japan*
- TP 241 **New workflow for contaminants screening in strawberries using high-resolution GC/Q-TOF and expanded accurate mass library of pesticides and environmental pollutants;** Sofia Nieto<sup>1</sup>; Anastasia Andrianova<sup>2</sup>; Jessica Westland<sup>2</sup>; Kai Chen<sup>1</sup>; Vadim Kalmeyer<sup>1</sup>; Yoshimasa Tsuno<sup>1</sup>; Li Sun<sup>1</sup>; Lei Tao<sup>1</sup>; Bruce Quimby<sup>2</sup>; Courtney Milner<sup>1</sup>; <sup>1</sup>*Agilent Technologies, Inc., Santa Clara, CA*; <sup>2</sup>*Agilent Technologies, Inc., Wilmington, DE*
- TP 246 **Time of Flight Secondary Ion Mass Spectrometry (TOF-SIMS) Imaging of Illicit Narcotics;** Greg Gillen<sup>1</sup>; Shin Muramoto<sup>2</sup>; Jennifer R. Verkouteren<sup>2</sup>; Edward Sisco<sup>2</sup>; <sup>1</sup>*National Institute of Standards and Technolgy, Gaithersburg, MD*; <sup>2</sup>*NIST, Gaithersburg, MD*
- TP 257 **Analysis of Synthetic Fentanyl Opioids in Serum using Captiva EMR-Lipid Sample Preparation by LC-QTOF;** Julie Cichelli; *Agilent Technologies, West Chester, PA*
- TP 259 **Screening, quantification and confirmation of fentanyl metabolite, N-[1-(2-phenethyl-4-piperidinyl)maloanilinic acid, in equine urine for doping control analysis by LC-MS/MS;** Youwen You<sup>1</sup>; Rachel M Proctor<sup>1</sup>; Fuyu Guan<sup>1</sup>; Jaclyn R Missanelli<sup>1</sup>; Xiaoqing Li<sup>1</sup>; Mary A Robinson<sup>1</sup>; <sup>1</sup>*University of Pennsylvania, Philadelphia, PA*
- TP 261 **Sub-minute Analysis for Samples of Forensic Applications;** Luis Cuadra-rodriguez<sup>1</sup>; Melissa Churley<sup>1</sup>; Lakshmi Krishnan<sup>1</sup>; Courtney Milner<sup>1</sup>; <sup>1</sup>*Agilent Technologies, Inc., Santa Clara, CA*
- TP 275 **Solely Concentrating on the Negative Aspects of Life;** Jordan Rabus<sup>1</sup>; Philippe Maître<sup>2</sup>; Benjamin J Bythell<sup>3</sup>; <sup>1</sup>*University of Missouri, St. Louis, Saint Louis, MO*; <sup>2</sup>*Laboratoire de Chimie Physique (UMR8000), CNRS, Univ. Paris-Sud, Université Paris-Saclay, Orsay, France*; <sup>3</sup>*University of Missouri - St. Louis, St. Louis, MO*
- TP 282 **Probing the Intrinsic Conformation of Anionic Uranyl Complexes Using IRMPD Spectroscopy and Quantum Chemical Calculations;** Scott D. Rissler<sup>1</sup>; Michael J. Van Stipdonk<sup>1</sup>; Luke Metzler<sup>1</sup>; Connor J Graca<sup>1</sup>; Irena Tatosian<sup>1</sup>; Amanda Bubas<sup>2</sup>; <sup>1</sup>*Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA*; <sup>2</sup>*University of Utah, Salt Lake City, UT*
- TP 299 **A Simple VOC Capturing Method Coupled with GC-MS;** Takeshi Furuhashi<sup>1</sup>; Shigenori Ota<sup>2</sup>; <sup>1</sup>*Anicom Specialty Medicinal Institute Inc, Tokyo, Japan*; <sup>2</sup>*GL science Inc, Iruma city, Saitama prefecture, Japan*
- TP 304 **Evaluation of matrix effect on pesticides in vegetables by GC-MS/MS;** Ge Yin<sup>1</sup>; Jun Fan<sup>2</sup>; <sup>1</sup>*Shimadzu China, Shanghai, China*; <sup>2</sup>*Shimadzu (China) Co., LTD., SHANGHAI, China*
- TP 319 **Epitope Mapping of Antibodies against Cobrotoxin and Cardiotoxin III by Hydrogen/Deuterium Exchange Mass Spectrometry;** Wei-Ya Chen<sup>1</sup>; Wang-Chou Sung<sup>2</sup>; Sung-fang Chen<sup>1</sup>; <sup>1</sup>*National Taiwan Normal University, Taipei, Taiwan*; <sup>2</sup>*National Health Research Institutes, Zhunan, Taiwan*
- TP 320 **Hydrogen Deuterium-Exchange Mass Spectrometry to Measure Nucleosome Dynamics;** Abigail A. Lemmon<sup>1</sup>; Geoffrey P. Dann<sup>1</sup>; Kelly R. Karch<sup>1</sup>; Benjamin A. Garcia<sup>1</sup>; <sup>1</sup>*University of Pennsylvania, Philadelphia, PA*
- TP 333 **Uncovering differential effects of IgG subclasses on whole DENV particles with hydrogen-deuterium exchange mass spectrometry;** Xin-Xiang Lim<sup>1</sup>; Ganesh S. Anand<sup>1</sup>; <sup>1</sup>*National University of Singapore, Singapore, Singapore*
- TP 337 **HDX-MS reveals allosteric changes in subtilisin serine protease upon inhibitor binding;** Daniel W Pedersen<sup>1,2</sup>; Jeppe C Mouritsen<sup>1</sup>; Stuart Pengelley<sup>3</sup>; Detlev Suckau<sup>3</sup>; Thomas J D Jørgensen<sup>2</sup>; Christian I Jørgensen<sup>1</sup>; <sup>1</sup>*Novozymes A/S, Bagsværd, Denmark*; <sup>2</sup>*University of Southern Denmark, Odense, Denmark*; <sup>3</sup>*Bruker Daltonik GmbH, Bremen, Germany*





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- TP 339 **Thermodynamic insight for the formulation optimization of a therapeutic antibody by HDX-MS analysis and nanoDSF;** Yoshitomo Hamuro<sup>1</sup>; Mehabaw Derebe<sup>1</sup>; Jennifer F. Nemeth-Seay<sup>1</sup>; <sup>1</sup>*Janssen Research and Development, Spring House, PA*
- TP 342 **Higher-Order Structural Analysis of Pro-Survival BAG-1S through HDX-MS;** Ozge Tatli<sup>1,2</sup>; Miray Turk<sup>1</sup>; Gizem Dinler Doganay<sup>1</sup>; <sup>1</sup>*Istanbul Technical University, Istanbul, Turkey*; <sup>2</sup>*Istanbul Medeniyet University, Istanbul, Turkey*
- TP 348 **Optimisation of a bottom-up strategy to detect biopharmaceuticals in 3D tumour models using MALDI-MSI;** Lucy E Flint<sup>1</sup>; Neil A Cross<sup>1</sup>; Laura M Cole<sup>1</sup>; David P Smith<sup>1</sup>; Malcolm R Clench<sup>1</sup>; <sup>1</sup>*Sheffield Hallam University, Sheffield, United Kingdom*
- TP 353 **A tool to visualize soil microbial community dynamics using mass spectrometry imaging and confocal microscopy;** Arunima Bhattacharjee<sup>1</sup>; Thomas W Wietsma<sup>1</sup>; Dusan Velickovic<sup>1</sup>; Sheryl L Bell<sup>1</sup>; Janet K Jansson<sup>1</sup>; Kirsten S Hofmockel<sup>1</sup>; Christopher R Anderton<sup>1</sup>; <sup>1</sup>*Pacific Northwest National Laboratory, Richland, WA*
- TP 380 **Keeping the shape of plant tissue for visualizing metabolite features of imaging mass spectrometry in Asparagus officinalis;** Ryo Nakabayashi<sup>1</sup>; Kei Hashimoto<sup>1</sup>; Kiminori Toyooka<sup>1</sup>; Tetsuya Mori<sup>1</sup>; Takashi Nirasawa<sup>2</sup>; Kazuki Saito<sup>1,3</sup>; <sup>1</sup>*RIKEN Center for Sustainable Resource Science, Yokohama, Japan*; <sup>2</sup>*Bruker Japan K. K., Yokohama, Japan*; <sup>3</sup>*Chiba University, Chuo-ku, Japan*
- TP 388 **Spatial lipidomics reveals altered lipid profiles in glomeruli of human diabetic kidney;** Guanshi Zhang<sup>1,2</sup>; Dušan Veličković<sup>3</sup>; Viktor Drel<sup>1,2</sup>; Sanjay Jain<sup>4</sup>; Shweta Bansal<sup>1,2</sup>; Manjeri A. Venkatachalam<sup>1</sup>; Hongping Ye<sup>1</sup>; Madesh Muniswamy<sup>1</sup>; Xianlin Han<sup>1</sup>; Ljiljana Paša-Tolić<sup>3</sup>; Theodore Alexandrov<sup>5,6</sup>; Christopher Anderton<sup>3</sup>; Kumar Sharma<sup>1,2</sup>; <sup>1</sup>*University of Texas Health-San Antonio, San Antonio, TX*; <sup>2</sup>*South Texas Veterans Health Care System, San Antonio, TX*; <sup>3</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>4</sup>*Washington University in St. Louis, St. Louis, MO*; <sup>5</sup>*European Molecular Biology Laboratory, Heidelberg, Germany*; <sup>6</sup>*University of California San Diego, La Jolla, CA*
- TP 396 **Spatial distribution of endogenous molecules in coffee bean by atmospheric pressure matrix-assisted laser desorption/ionization mass spectrometry imaging;** Honggang Nie<sup>1</sup>; Chenglong Dong<sup>2</sup>; Yehua Han<sup>2</sup>; Huwei Liu<sup>1</sup>; <sup>1</sup>*Beijing National Laboratory for Molecular Sciences, Peking University, Beijing, China*; <sup>2</sup>*State Key Laboratory of Heavy Oil Processing, China University of Petroleum, Beijing, China*
- TP 403 **MALDI Imaging Mass Spectrometry as a Tool to Evaluate Levels of ATP and its Metabolites in Mouse Tumor Models;** Stephanie Dale<sup>1</sup>; Cristine Quiason-Huynh<sup>2</sup>; <sup>1</sup>*Genentech, South San Francisco, CA*; <sup>2</sup>*Genentech, Inc., South San Francisco, CA*
- TP 408 **Next-Generation Software for Visualization and Computational Analysis of High-performance Ion Mobility Molecular Imaging Data;** Lukasz Migas<sup>1</sup>; Jeffrey M. Spraggins<sup>2,3</sup>; Richard M. Caprioli<sup>2,3</sup>; Perdita E. Barran<sup>4,5</sup>; Raf Van de Plas<sup>1,3</sup>; <sup>1</sup>*Delft University of Technology, Delft, Netherlands*; <sup>2</sup>*Vanderbilt University, Nashville, TN*; <sup>3</sup>*Vanderbilt Mass Spectrometry Research Center and Department of Biochemistry, Nashville, TN*; <sup>4</sup>*University of Manchester, Manchester, United Kingdom*; <sup>5</sup>*Manchester Institute of Biotechnology, University of Manchester, United Kingdom*
- TP 409 **Automatic molecular annotation of mass spectrometry imaging data;** Jan H. Kobarg<sup>1</sup>; Nikolas Kessler<sup>2</sup>; Wiebke Timm<sup>2</sup>; Janina Oetjen<sup>2</sup>; Klaus Steinhorst<sup>1</sup>; Stefan Schiffler<sup>1</sup>; Shannon Cornett<sup>3</sup>; Aiko Barsch<sup>2</sup>; Heiko Neuweger<sup>2</sup>; Alice Ly<sup>2</sup>; Dennis Trede<sup>1</sup>; <sup>1</sup>*SCiLS, Bremen, Germany*; <sup>2</sup>*Bruker Daltonik GmbH, Bremen, Germany*; <sup>3</sup>*Bruker Daltonics Inc., Billerica, MA*
- TP 428 **Conotoxin Exploitation from Conus betulinus Using an Integrated Approach of Transcriptomic and Peptidomics;** He yanbin<sup>1</sup>; Lin zhilong<sup>1</sup>; Luo Xing<sup>1</sup>; Ren zhe<sup>1</sup>; Roy Bhaskar<sup>1</sup>; Qi Da<sup>1</sup>; Liu Siqi<sup>1</sup>; <sup>1</sup>*BGI-Shenzhen, Shenzhen, China*
- TP 432 **A multi-omics approach to linking proteomic profiles and metabolomic phenotypes provides insight into colorectal cancer cell metabolism;** Peter Doubleday<sup>1</sup>; Ioanna Ntai<sup>2</sup>; Luca Fornelli<sup>3</sup>; Emily Boja<sup>4</sup>;



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- Henry Rodriguez<sup>4</sup>; Neil L Kelleher<sup>1</sup>; <sup>1</sup>*Northwestern University, Evanston*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>3</sup>*The University of Oklahoma, Norman, OK*; <sup>4</sup>*Office of Cancer Clinical Proteomics Research, NIH, Bethesda, MD*
- TP 434 **Evaluating Machine Learning Methods Capable of Handling Missing Values for Protein Biomarker Studies;** David Nusinow<sup>1</sup>; John Szpyt<sup>1</sup>; Steven P Gygi<sup>1</sup>; <sup>1</sup>*Harvard Medical School, Boston, MA*
- TP 437 **pmartR: Software for Quality Control and Statistics Robust to Missing Data for Mass Spectrometry-based Biological Data;** Lisa Bramer<sup>1</sup>; Kelly G. Stratton<sup>1</sup>; Bobbie-jo M. Webb-robertson<sup>1</sup>; Lee Ann McCue<sup>1</sup>; Bryan Stanfill<sup>1</sup>; Daniel Claborne<sup>1</sup>; Allison M. Thompson<sup>1</sup>; Iobani Godinez<sup>1</sup>; <sup>1</sup>*Pacific Northwest National Laboratory, Richland, WA*
- TP 439 **Integrated Omics Analysis Across 32 Human Tissues;** Lihua Jiang<sup>1</sup>; Meng Wang<sup>2</sup>; Shin Lin<sup>3</sup>; Ruiqi Jian<sup>2</sup>; Joanne Chan<sup>2</sup>; Xiao Li<sup>2</sup>; Huaying Fang<sup>2</sup>; Hua Tang<sup>2</sup>; Michael Snyder<sup>2</sup>; <sup>1</sup>*Stanford University, Stanford, CA*; <sup>2</sup>*Stanford University, Palo Alto, CA*; <sup>3</sup>*University of Washington, Seattle, WA*
- TP 450 **Profiling Agrochemical Residues in Produce via Paper Cone Spray Ionization and Portable Instrumentation;** Alyssa J. Gasa<sup>1</sup>; Makoy R. Overfelt<sup>1</sup>; Christopher Mulligan<sup>2</sup>; <sup>1</sup>*Illinois state university, Normal, IL*; <sup>2</sup>*Illinois State University, Normal, IL*
- TP 465 **Paper Spray Ionization Mass Spectrometry of Sebum Samples: A Step Towards Rapid, Early Diagnosis of Parkinson's Disease;** Depanjan Sarkar<sup>1</sup>; Drupad Trivedi<sup>1</sup>; Caitlin Walton-Doyle<sup>1</sup>; Joy Milne<sup>1</sup>; Eleanor Sinclair<sup>1</sup>; Monty Silverdale<sup>1</sup>; Perdita Barran<sup>1</sup>; <sup>1</sup>*University of Manchester, Manchester, United Kingdom*
- TP 467 **Enhanced Charge Detection Mass Spectrometry Precision with a Low-Noise Amplifier Without a Feedback Resistor;** Aaron R Todd<sup>1</sup>; Andrew W Alexander<sup>1</sup>; Martin F Jarrold<sup>1</sup>; <sup>1</sup>*Indiana University, Bloomington, IN*
- TP 472 **Distance-of-Flight Mass Spectrometry using a Semiconductor Ion Detector Array;** Steven Ray; *University at Buffalo, SUNY, Buffalo, NY*
- TP 491 **Microsampling with Cotton Threads and Direct Analysis via Ambient Mass Spectrometry;** Devin Swiner<sup>1</sup>; Sierra Jackson<sup>1</sup>; George R. Durisek<sup>1</sup>; Bridget K. Walsh<sup>1</sup>; Yaman Kouatli<sup>1</sup>; Abraham K. Badu-Tawiah<sup>1</sup>; <sup>1</sup>*The Ohio State University, Columbus, OH*
- TP 501 **Analysis of Specific Metal Binding to Alpha-Synuclein with Collisional Induced Unfolding;** Neil R. Quebbemann<sup>1</sup>; Joseph A. Loo<sup>1</sup>; <sup>1</sup>*University of California Los Angeles, Los Angeles, CA*
- TP 505 **An investigation into the use of cyclic ion mobility for the separation of biopharmaceutical peptide and protein modifications;** Jim Langridge<sup>1</sup>; Henry Shion<sup>2</sup>; Martin Palmer<sup>3</sup>; Weibin chen<sup>2</sup>; Dale A Cooper-shepherd<sup>3</sup>; <sup>1</sup>*Waters Corporation, Wilmslow, United Kingdom*; <sup>2</sup>*Waters Corporation, Milford, MA*; <sup>3</sup>*Waters Corporation, Wilmslow, United Kingdom*
- TP 508 **Direct Identification of Endogenous Ligands Bound to Specific Protein Conformations Using Multistage Gas Phase Separation on a Cyclic-Mobility Mass Spectrometer;** Idlir Liko<sup>1</sup>; Joseph F Gault<sup>2</sup>; Martin Palmer<sup>3</sup>; Dale A Cooper-shepherd<sup>3</sup>; Jakub Ujma<sup>3</sup>; Carol V. Robinson<sup>2</sup>; <sup>1</sup>*OMass Therapeutics, Oxford, United Kingdom*; <sup>2</sup>*Oxford University, Oxford, United Kingdom*; <sup>3</sup>*Waters Corporation, Wilmslow, United Kingdom*
- TP 539 **A New HILIC LC/Q-TOF Metabolomics Method with Biologically Important Isomer Separation and Broad Coverage of Metabolite Classes;** Yuqin Dai<sup>1</sup>; Jordy J. Hsiao<sup>1</sup>; <sup>1</sup>*Agilent Technologies, Santa Clara, CA*
- TP 540 **Development of more reproducible and sensitive polar metabolomics methods;** Sara Violante<sup>1</sup>; Hardik Shah<sup>1</sup>; Yuqin Dai<sup>2</sup>; Steven M Fischer<sup>2</sup>; Justin R Cross<sup>1</sup>; <sup>1</sup>*Memorial Sloan Kettering Cancer Center, New York, NY*; <sup>2</sup>*Agilent Technologies, Inc., Santa Clara, CA*
- TP 545 **Volatile Metabolites Monitoring of Gut Microbiota Using Secondary Electrospray Based Mass Spectrometry Techniques- a Tale of Two Approaches;** Haorong Li<sup>1</sup>; Mengyang Xu<sup>1</sup>; Jiangjiang (Chris) Zhu<sup>2</sup>; <sup>1</sup>*Miami University, Oxford, OH*; <sup>2</sup>*The Ohio State University, Columbus, OH*



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- TP 546 **Revealing the Changes in Pulmonary Arterial Smooth Muscle Cells in Patient by Using Multi-Omics Approach;** Dan Li<sup>1,2,3</sup>; Songjie Chen<sup>4</sup>; Marlene Rabinovitch<sup>1,2,3</sup>; Michael Snyder<sup>4</sup>; <sup>1</sup>*Department of Pediatrics, Stanford University School of Medicine, Stanford, CA 94305*; <sup>2</sup>*Stanford Cardiovascular Institute, Stanford University, Stanford, CA 94305*; <sup>3</sup>*Vera Moulton Wall Center for Pulmonary Vascular Diseases, Stanford University School of Medicine, Stanford, CA 94305*; <sup>4</sup>*Department of Genetics, Stanford University School of Medicine, Stanford, CA 94305*
- TP 552 **Fast detection of pesticides and drugs removed from waste water by plants using Flow Injection Analysis Magnetic Resonance Mass Spectrometry;** Claire Villette<sup>1</sup>; Matthias Witt<sup>2</sup>; Aiko Barsch<sup>2</sup>; Louis Maljers<sup>3</sup>; Dimitri Heintz<sup>4</sup>; <sup>1</sup>*University of Strassbourg, Strassbourg, France*; <sup>2</sup>*Bruker Daltonik GmbH, Bremen, Germany*; <sup>3</sup>*Bruker Daltonics Inc., Billerica, MA*; <sup>4</sup>*University of Strasbourg, Strasbourg, France*
- TP 555 **Profiling weaning piglet serum metabolomic affected by acute exposure of high concentrations atmospheric hydrogen sulfide;** Zhen Liu<sup>1</sup>; Qingshi Meng<sup>1</sup>; Qixiang Miao<sup>1</sup>; Yanjiao Xie<sup>1</sup>; Hongfu Zhang<sup>1</sup>; Xiangfang Tang<sup>1</sup>; <sup>1</sup>*Institute of Animal Science, Chinese Academy of Agricultural Sciences, Beijing, China*
- TP 564 **Multi-omic Discovery of Metabolic Rewiring in Triple-negative Breast Cancer Following Mitochondrial Folate Transport Ablation: Strategy to Reveal Drug-targetable Synthetic Lethalities;** Qiuying Chen<sup>1</sup>; Joshua B Zuk<sup>1</sup>; miller A Christine<sup>2</sup>; Steven M Fischer<sup>2</sup>; Steven Gross<sup>1</sup>; <sup>1</sup>*Weill Medical College of Cornell, New York, NY*; <sup>2</sup>*Agilent Technologies, Inc., Santa Clara, CA*
- TP 569 **Global Quantification of Proteome and Phosphoproteome Revealed Novel Cellular Signaling Mechanisms Responsive to Hypoxia and Iron Deficiency;** Luke Erber<sup>1</sup>; Yao Gong<sup>1</sup>; Maolin Tu<sup>1</sup>; Phu Tran<sup>1</sup>; Yue Chen<sup>1</sup>; <sup>1</sup>*University of Minnesota, Minneapolis, MN*
- TP 573 **Quantitative, comprehensive multi-pathway signaling analysis using an optimized phosphopeptide enrichment method combined with an internal standard triggered targeted MS assay;** Bhavin Patel<sup>1</sup>; Penny Jensen<sup>1</sup>; Aaron S. Gajadhar<sup>2</sup>; Sebastien Gallien<sup>3</sup>; Jae Choi<sup>1</sup>; Romain Huguette<sup>2</sup>; Graeme Mcalister<sup>2</sup>; Derek Bailey<sup>2</sup>; Shannon Eliuk<sup>2</sup>; Markus Kellmann<sup>4</sup>; Tabiwang N. Arrey<sup>4</sup>; Alexander Harder<sup>4</sup>; Andreas Huhmer<sup>2</sup>; Kay Opperman<sup>1</sup>; John C Rogers<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, Rockford, IL*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>3</sup>*Thermo Fisher Scientific, Precision Medicine Science Center, Cambridge, MA*; <sup>4</sup>*Thermo Fisher Scientific, Bremen, Germany*
- TP 576 **Proteomic and Phosphoproteomic Network analysis in Alzheimer's Disease;** Lingyan Ping<sup>1,2</sup>; Eric B Dammer<sup>1,2</sup>; Duc M Duong<sup>2,3</sup>; Marla Gearing<sup>2</sup>; James J. Lah<sup>2,4</sup>; Allan I. Levey<sup>2,4</sup>; Nicholas T. Seyfried<sup>1,2,4</sup>; <sup>1</sup>*Department of Biochemistry, Emory University, Atlanta, GA*; <sup>2</sup>*Center for Neurodegenerative Diseases, Emory School of Medicine, Atlanta, GA*; <sup>3</sup>*Department of Biochemistry, Emory University, Atlanta, Georgia*; <sup>4</sup>*Department of Neurology, Emory University, Atlanta, GA*
- TP 582 **Immunocapture-LC/MS and LBA-based assays as complementary and orthogonal tools for developing fusion protein therapeutics;** Susan Chen; *Takeda Pharmaceuticals, Inc., Cambridge, MA*
- TP 584 **Impact of Endogenous Biotin on Streptavidin Based Hybrid LBA-LC/MS Assays for Biotherapeutics;** Eric Ma<sup>1</sup>; Moucun Yuan<sup>1</sup>; William R Mylott Jr<sup>1</sup>; <sup>1</sup>*PPD, Richmond, VA*
- TP 585 **Biotransformation of Challenging New Modalities –Characterization and Quantitation of Antibody Variant Fragmentation using Affinity Capture coupled to LC-MS or CE-LIF;** Cong Wu<sup>1</sup>; William Sawyer<sup>1</sup>; Phillip Chu<sup>1</sup>; Neha Srikumar<sup>2</sup>; Nga Tang<sup>1</sup>; Pamela Chan<sup>1</sup>; Gloria Meng<sup>1</sup>; Brian Roper<sup>3</sup>; Thomas Niedringhaus<sup>3</sup>; John Tran<sup>1</sup>; <sup>1</sup>*Biochemical and Cellular Pharmacology, Genentech, Inc., South San Francisco, CA*; <sup>2</sup>*University of Pennsylvania, Philadelphia, PA*; <sup>3</sup>*Protein Analytical Chemistry, Genentech, Inc., South San Francisco, California*
- TP 586 **Multi Attribute Monitoring in Therapeutic glycoprotein process development: Benchmark of different sample preparation, mass spectrometry platform and data processing software;** Bertaccini Diego; *Merck KGaA Darmstadt, Germany, Corsier-sur-Vevey, Switzerland*



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- TP 589 **Employing the MS-based Multi-attribute Method (MAM) for Automated Quality Monitoring of Biotherapeutics;** John N McCarter<sup>1</sup>; Joe Shambaugh<sup>2</sup>; Aude Tartiere<sup>3</sup>; Albert Van Wyk<sup>4</sup>; Cassandra Wigmore<sup>5</sup>; Peter Haberl<sup>6</sup>; <sup>1</sup>*Genedata, Inc., Lexington, MA*; <sup>2</sup>*Genedata Inc, Lexington, MA, USA, Lexington, Massachusetts*; <sup>3</sup>*Genedata, San Francisco, CA*; <sup>4</sup>*Genedata Ltd, Cambridge, UK, Cambridge, United Kingdom*; <sup>5</sup>*Genedata AG, Basel, Switzerland, Basel, Switzerland*; <sup>6</sup>*Genedata GmbH, Munich, Germany, Munich, Germany*
- TP 591 **A high resolution accurate mass multi-attribute method for critical quality attribute monitoring and new peak detection;** Haichuan Liu<sup>1</sup>; John Rontree<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*
- TP 592 **Monitoring Multiple Attributes of Biotherapeutics at Peptide Level using a Single Quadrupole LC/MS for Quality Control;** Linfeng Wu<sup>1</sup>; Lisa Zang<sup>1</sup>; Guannan Li<sup>1</sup>; Ning Tang<sup>1</sup>; Henry Shu<sup>2</sup>; <sup>1</sup>*Agilent Technologies, Santa Clara, CA*; <sup>2</sup>*Agilent Technologies, Inc., Santa Clara, CA*
- TP 594 **Mass Spectrometric Evaluation of Host Cell Protein Patterns in Biopharmaceutical Products;** Daniel Michael Waldera-Lupa<sup>1</sup>; Thomas Flad<sup>1</sup>; Andreas Dittmar<sup>1</sup>; Heiner Falkenberg<sup>1</sup>; Roland Moussa<sup>1</sup>; <sup>1</sup>*Protagen Protein Services, Dortmund, Germany*
- TP 595 **Pre-clinical estimation of cetuximab using nano-surface and molecular orientation limited (nSMOL) proteolysis and LC-MS/MS;** Deepti Bhandarkar<sup>1</sup>; Rashi Kochhar<sup>1</sup>; Shailendra Rane<sup>1</sup>; Shailesh Damale<sup>1</sup>; Ashutosh Shelar<sup>1</sup>; Purushottam Sutar<sup>1</sup>; Anant Lohar<sup>1</sup>; Bhaumik Trivedi<sup>1</sup>; Navin Devadiga<sup>1</sup>; Ajit Datar<sup>1</sup>; Pratap Rasam<sup>1</sup>; Jitendra Kelkar<sup>1</sup>; <sup>1</sup>*Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*
- TP 597 **Investigation of Tissue Distributions of Therapeutic Monoclonal Antibody With Cassette Dosing Strategy and Novel LC/MS Based Method;** Jie Pu<sup>1</sup>; Shihan Huo<sup>1</sup>; Chao Xue<sup>1</sup>; Ming Zhang<sup>1, 2</sup>; Jun Qu<sup>1, 2</sup>; <sup>1</sup>*SUNY, at Buffalo, Buffalo, NY*; <sup>2</sup>*New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, New York*
- TP 599 **Application of Top Down Degradomics to Guide Development of Stable Antibody Variants;** Phillip Chu<sup>1</sup>; christopher Davies<sup>2</sup>; Cong Wu<sup>2</sup>; Tangsheng Yi<sup>2</sup>; James Koerber<sup>2</sup>; John C. Tran<sup>2</sup>; <sup>1</sup>*Genentech Inc., South San Francisco, CA*; <sup>2</sup>*Genentech, South San Francisco, CA*
- TP 603 **An Integrated LC-MS Platform for Monitoring Quality Attributes of Biotherapeutic Products;** Chengfeng Ren<sup>1</sup>; Frank Macchi<sup>2</sup>; Monica Sadek<sup>2</sup>; Benjamin Moore<sup>2</sup>; <sup>1</sup>*Genentech, South San Francisco, CA*; <sup>2</sup>*Genentech Inc., South San Francisco, CA*
- TP 610 **Analysis of aggregation-prone full-length antibodies using FPOP-LC-MS/MS;** Owen Cornwell<sup>1</sup>; Nicholas J Bond<sup>2</sup>; Sheena E Radford<sup>1</sup>; Alison E Ashcroft<sup>1</sup>; <sup>1</sup>*University of Leeds, Leeds, United Kingdom*; <sup>2</sup>*MedImmune, Cambridge, United Kingdom*
- TP 616 **Identifying early production truncated drug candidates by Top-Down mass spectrometry;** Zhe Zhang; *Novartis, Cambridge, MA*
- TP 620 **Novel analytical paradigm for accurate characterization and routine monitoring of deamidation and succinimide intermediate in biotherapeutic proteins;** Sergei Saveliev<sup>1</sup>; Mingyan Cao<sup>2</sup>; Sri Hari Raju Mulagapati<sup>2</sup>; Bhargavi Vemulapati<sup>2</sup>; Jihong Wang<sup>2</sup>; Alan Hunter<sup>2</sup>; Marjeta Urh<sup>1</sup>; Dengfeng Liu<sup>2</sup>; <sup>1</sup>*Promega Corporation, Madison, WI*; <sup>2</sup>*MedImmune, Gaithersburg, MD*
- TP 626 **Protein phosphorylation landscape of mouse spermatids during spermiogenesis;** Yan Li<sup>1</sup>; Yiwei Cheng<sup>1</sup>; Tianyu Zhu<sup>1</sup>; Hao Zhang<sup>1</sup>; Hui Zhu<sup>1</sup>; Xuejiang Guo<sup>1</sup>; <sup>1</sup>*Nanjing Medical University, Nanjing, China*
- TP 631 **Phosphoproteomic analyses of multiple species of snakes provides insight into the regulation of intestinal function and regeneration;** Abu Hena M Kamal<sup>1</sup>; Blair Perry<sup>1</sup>; Todd Castoe<sup>1</sup>; Stephen M. Secor<sup>2</sup>; Saiful M. Chowdhury<sup>1</sup>; <sup>1</sup>*University of Texas at Arlington, Arlington, TX*; <sup>2</sup>*University of Alabama, Tuscaloosa, AL*
- TP 638 **Characterization of S-Nitrosylation in Aged Rabbit using Oxidized Cysteine-selective cPILOT;** Katarena Ford; *Vanderbilt University, Nashville, TN*



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- TP 645 **Orthogonal Approaches for Released N-Glycan Characterization and Quantification;** Sean Mccarthy<sup>1</sup>; Zoe Zhang<sup>2</sup>; Elliott Jones<sup>2</sup>; <sup>1</sup>SCIEX, Framingham, MA; <sup>2</sup>Sciex, Redwood City, CA
- TP 648 **Dynamic Bovine Milk Proteome Alterations during Staphylococcus aureus Infection in Subclinical and Clinical Mastitis;** Kiran Ambatipudi<sup>1</sup>; Sudipa Maity<sup>1</sup>; Debiprasanna Das<sup>2</sup>; <sup>1</sup>Indian Institute of Technology Roorkee, Roorkee, India; <sup>2</sup>College of Veterinary Science and Animal Husbandry, Bhubaneswar, India
- TP 649 **Identifying the molecular mechanisms of sex-specific severity of the Middle East Respiratory Syndrome Coronavirus (MERS-CoV) using proteomics;** Natarajan Bhanu<sup>1</sup>; Simone Sidoli<sup>1</sup>; Ranran Wu<sup>1</sup>; Neeltje van Doremalen<sup>2</sup>; Vincent Munster<sup>2</sup>; Angela Rasmussen<sup>3</sup>; Benjamin A. Garcia<sup>4</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA; <sup>2</sup>National Institutes of Health, Rocky Mountain Laboratories, Hamilton, MT; <sup>3</sup>Columbia University Mailman School of Public Health, New York City, NY; <sup>4</sup>University of Pennsylvania, Philadelphia, PA
- TP 656 **Comprehensive analysis of the human cytomegalovirus interactome to identify key hubs of protein degradation;** Luis Nobre<sup>1</sup>; Katie Nightingale<sup>1</sup>; Benjamin J Ravenhill<sup>1</sup>; Robin Antrobus<sup>1</sup>; Gavin W.G. Wilkinson<sup>2</sup>; Richard J Stanton<sup>2</sup>; Edward L Huttlin<sup>3</sup>; Michael Weekes<sup>1</sup>; <sup>1</sup>University of Cambridge, Cambridge, United Kingdom; <sup>2</sup>University of Cardiff, Cardiff, United Kingdom; <sup>3</sup>Harvard Medical School, Boston, MA
- TP 659 **Impaired Degradation Dynamics of Synaptic Vesicle Machinery in APPKI Mice;** Nalini R Rao<sup>1</sup>; Ewa Bomba-warczak<sup>1</sup>; Timothy Hark<sup>1</sup>; Jeffrey N. Savas<sup>1</sup>; <sup>1</sup>Northwestern University, Chicago, IL
- TP 660 **Mass spectrometry in the development of better coagulation tests: quantitation and proteoform characterization of antithrombin;** Renee Ruhaak<sup>1</sup>; Fred P.H.T.M. Romijn<sup>1</sup>; Mervin Pieterse<sup>1</sup>; Jan Nouta<sup>1</sup>; Nico Smit<sup>1</sup>; Elena Dominguez-Vega<sup>1</sup>; Yuri E.M. van der Burgt<sup>1</sup>; Manfred Wuhrer<sup>1</sup>; Christa M. Cobbaert<sup>1</sup>; <sup>1</sup>LUMC, Leiden, Netherlands
- TP 662 **A Direct Computational Approach to the Analysis of Multiply Charged Biomolecules and Their Modifications with Electrospray Mass Spectrometry;** Ning Zhang<sup>1</sup>; Shundi Shi<sup>2</sup>; Shenglong Zhang<sup>1</sup>; David Good<sup>3</sup>; Don Kuehl<sup>4</sup>; Yongdong Wang<sup>4</sup>; <sup>1</sup>Department of Life Sciences, New York Institute of Technology, New York, NY; <sup>2</sup>Department of Chemical Engineering, Columbia University, New York, NY; <sup>3</sup>Covance Laboratories Inc., Madison, WI; <sup>4</sup>Cerno Bioscience, Norwalk, CT
- TP 668 **Application of Probabilistic Information Retrieval for Ultra Rapid Peptide Sequencing Utilizing Comprehensive Protein Isoform Databases;** Jeffrey J. Jones<sup>1</sup>; Ryan Benz<sup>1</sup>; <sup>1</sup>SoCal Bioinformatics Inc., Montrose, CA
- TP 670 **Single cell proteomic analysis using PASEF;** Catherine C L Wong; Center for Precision Medicine Multiomics Research, Peking University, Beijing, China
- TP 673 **Ultra-fast proteomics enabled by Scanning SWATH and high-flow chromatography;** Christoph B Messner<sup>1</sup>; Vadim Demichev<sup>2,3</sup>; Spyros Vernardis<sup>3</sup>; Nic Bloomfield<sup>4</sup>; Gordana Ivosev<sup>4</sup>; Frasn Wasim<sup>4</sup>; Stephen Tate<sup>4</sup>; Kathryn Lilley<sup>2</sup>; Markus Ralser<sup>3,5</sup>; <sup>1</sup>Francis Crick Institute, London, United Kingdom; <sup>2</sup>Department of Biochemistry, University of Cambridge, Cambridge, United Kingdom; <sup>3</sup>The Francis Crick Institute, London, United Kingdom; <sup>4</sup>SCIEX, Concord, ON; <sup>5</sup>Charité, Berlin, Germany
- TP 679 **Cysteine Directed Proteolysis for Middle Down Proteomics;** Joe R. Cannon<sup>1</sup>; J. Wade Harper<sup>2</sup>; Mark Cancilla<sup>1</sup>; <sup>1</sup>Merck & Co., Inc., West Point, PA; <sup>2</sup>Harvard Medical School, Boston, MA
- TP 683 **Comprehensive evaluation of shotgun proteomics using Thermo Scientific Orbitrap Fusion Lumos Mass Spectrometer with FAIMS Pro Interface;** Yue Zhou<sup>1</sup>; Min Huang<sup>1</sup>; Xiangyun Yang<sup>1</sup>; Mo Hu<sup>1</sup>; Jing Li<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Shanghai, China
- TP 687 **Plasma proteomics goes high throughput;** Raphael A Heilig<sup>1</sup>; Thomas Kosinski<sup>2</sup>; Yuxin Mi<sup>3</sup>; Katie L Burnham<sup>3</sup>; Julian C Knight<sup>3</sup>; Heiner Koch<sup>2</sup>; Roman Fischer<sup>1</sup>; <sup>1</sup>Target Discovery Institute, Nuffield Department of Medicine, University of Oxford, Oxford, United Kingdom; <sup>2</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>3</sup>Wellcome Centre for Human Genetics, University of Oxford, Oxford, United Kingdom



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- TP 691 **A labeling enrichment method based on synergistic and reversible covalent interactions forselenoproteinanalysis;** Qingshi Meng<sup>1</sup>; Hongfu zhang<sup>1</sup>; Xiaohui feng<sup>1</sup>; <sup>1</sup>*Institute of Animal Sciences, CAAS, Beijing, China*
- TP 697 **Arc-negative extracellular vesicles promote bidirectional synaptic communication through CaMKII;** Yi-Zhi Wang<sup>1</sup>; Samuel N. Smukowski<sup>1</sup>; Claire Piochon<sup>1</sup>; Ewa Bomba-warczak<sup>1</sup>; Qionger He<sup>1</sup>; Stacy A. Marshall<sup>1</sup>; Elizabeth T. Bartom<sup>1</sup>; Ali Shilatifard<sup>1</sup>; Anis Contractor<sup>1</sup>; Jeffrey N. Savas<sup>1</sup>; <sup>1</sup>*Northwestern University, Chicago, IL*
- TP 705 **Spatially-Resolved Neuroproteomics with IonStar Reveals Differential Landscapes of Signal Transduction Dysregulation in a Rat Ischemic Stroke Model;** Shichen Shen<sup>1</sup>; Min Ma<sup>2</sup>; Ming Zhang<sup>1</sup>; David Poulsen<sup>1</sup>; Jun Qu<sup>1</sup>; <sup>1</sup>*University at Buffalo, Buffalo, NY*; <sup>2</sup>*Roswell Park Comprehensive Cancer Center, Buffalo, NY*
- TP 710 **Isobaric reporter ion cascades for high capacity multiplexing;** Brian Erickson<sup>1</sup>; Ryan Kunz<sup>1</sup>; Steven P Gygi<sup>2</sup>; Craig Braun<sup>1</sup>; <sup>1</sup>*IQ Proteomics LLC, Cambridge, MA*; <sup>2</sup>*Harvard Medical School, Boston, MA*
- TP 729 **Direct Thermal Proteome Profiling using Quantitative Top-Down Proteomics;** Kellye A Cupp-sutton<sup>1</sup>; Zhe Wang<sup>1</sup>; Si Wu<sup>1</sup>; <sup>1</sup>*University of Oklahoma, Norman*
- TP 733 **Deep Intact Proteome Quantification using Protein-Level Tandem Mass Tag (TMT) Labeling and online 2D Liquid chromatography;** Dahang Yu<sup>1</sup>; Zhe Wang<sup>1</sup>; Kellye A Cupp-sutton<sup>1</sup>; Kenneth Smith<sup>2</sup>; Xiaowen Liu<sup>3</sup>; Si Wu<sup>1</sup>; <sup>1</sup>*University of Oklahoma, Norman, OK*; <sup>2</sup>*Oklahoma Medical Research Foundation, Oklahoma City, OK*; <sup>3</sup>*Indiana University-Purdue University Indianapolis, Indianapolis, IN*
- TP 734 **Investigating the stability of linear polyacrylamide coating for capillary zone electrophoresis-tandem mass spectrometry-based top-down proteomics;** Tian Xu; *Michigan State University, East Lansing, MI*
- TP 738 **Interpretation of Mass Spectrometric Data for Structure Elucidation of a New Endogenous Organosulfur Metabolite;** Qibo Zhang<sup>1</sup>; Lisa A. Ford<sup>1</sup>; Anne M. Evans<sup>1</sup>; Douglas R. Toal<sup>1</sup>; <sup>1</sup>*Metabolon, Morrisville, NC*
- TP 742 **Investigation and Profiling of Organic Solvent Based Lithium Ion Battery Electrolytes and the Decomposition products;** Nan Hu; *Agilent Technologies, Beijing, China*
- TP 744 **Identification of Degradation Products of Epirubicin based on multiple heart-cut2D LC-Q TOF;** Yaping Zhang<sup>1</sup>; Hui Ouyang<sup>2</sup>; Congfang Lai<sup>3</sup>; <sup>1</sup>*Agilent Technologies, Shanghai, China*; <sup>2</sup>*Jiangxi University of Traditional Chinese Medicine, Nanchang, China*; <sup>3</sup>*Agilent Technologies(China) Co. Ltd., Beijing, China*
- TP 746 **Simplified approach for structural elucidation and quantitation for pharmaceutical API and related impurities using Q-TOF;** Purushottam Janardan Sutar<sup>1</sup>; Shailendra Rane<sup>1</sup>; Shailesh Damale<sup>1</sup>; Rashi Kochhar<sup>1</sup>; Deepti Bhandarkar<sup>1</sup>; Anant Lohar<sup>1</sup>; Ashutosh Shelar<sup>1</sup>; Bhaumik Trivedi<sup>1</sup>; Navin Devadiga<sup>1</sup>; Ajit Datar<sup>1</sup>; Pratap Rasam<sup>1</sup>; Jitendra Kelkar<sup>1</sup>; <sup>1</sup>*Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*
- TP 753 **Selective gas-phase mass tagging via ion/molecule reactions combined with single analyzer neutral loss scans to probe pharmaceutical mixtures;** Dalton T. Snyder<sup>1</sup>; Lucas J. Szalwinski<sup>1</sup>; Alice Pilo<sup>2</sup>; Nina K. Jarrah<sup>2</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*Merck & Co., Inc., Rahway, NJ*
- TP 759 **Interferon Stimulated Gene 15 controls phagosome maturation;** Frederic Lamoliatte<sup>1</sup>; Tiaan Heunis<sup>1</sup>; Anetta Svitorka Hartlova<sup>1</sup>; Matthias Trost<sup>1</sup>; <sup>1</sup>*ICAMB, Newcastle University, Newcastle Upon Tyne, United Kingdom*
- TP 760 **Multi-Omics profiling and customized gRNA library CRISPR-CAS9 genomic screening identify cancer vulnerabilities in brain tumors;** Hong Wang<sup>1</sup>; Mingming Niu<sup>2</sup>; Timothy I. Shaw<sup>2</sup>; yuxin Li<sup>2</sup>; Ji-Hoon cho<sup>2</sup>; Anthony High<sup>1</sup>; Vishwajeeth Pagala<sup>2</sup>; Xusheng Wang<sup>2</sup>; Junmin Peng<sup>1</sup>; <sup>1</sup>*St. Jude Children's Research Hospital, Memphis, TN*; <sup>2</sup>*St. Jude children's Research hospi, Memphis, TN*
- TP 763 **A novel HLA-peptide profiling workflow called MAPTAC (Mono-Allelic-Purification-with-Tagged-Allele-Constructs) leverages mass spectrometry to improve neoantigen prediction;** Daniel Rothenberg<sup>1</sup>; Jennifer Abelin<sup>1</sup>; Dominik Barthelme<sup>1</sup>; Rob C Oslund<sup>1</sup>; Amanda L Creech<sup>1</sup>; Tyler Colson<sup>1</sup>; Scott P



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- Goulding<sup>1</sup>; Lia R Serrano<sup>1</sup>; Chris Mcgann<sup>1</sup>; Ying S Ting<sup>1</sup>; Yusuf Nasrullah<sup>1</sup>; Janani Sridar<sup>1</sup>; Dewi Harjanto<sup>1</sup>; Matt Malloy<sup>1</sup>; Christina Kuksin<sup>1</sup>; Joel Greshock<sup>1</sup>; Terri A Addona<sup>1</sup>; Michael S Rooney<sup>1</sup>; <sup>1</sup>*Neon Therapeutics, Cambridge, MA*
- TP 766 **Metagenomic-based Metaproteomic Functional Characterization of the Sargasso Sea in a Three Year Time Series Dataset;** Mak Saito<sup>1</sup>; Brian Searle<sup>2</sup>; Dawn Moran<sup>3</sup>; Jaci Saunders<sup>3</sup>; Noelle Held<sup>3</sup>; Chris Dupont<sup>4</sup>; Rod Johnson<sup>5</sup>; Matthew McIlvin<sup>3</sup>; <sup>1</sup>*Woods Hole Oceanographic Inst., Woods Hole Ma 02543, MA;* <sup>2</sup>*Institute for Systems Biology, Seattle, Washington;* <sup>3</sup>*Woods Hole Oceanographic Institution, Woods Hole;* <sup>4</sup>*J. Craig Venter Institute, La Jolla, CA;* <sup>5</sup>*Bermuda Institute of Ocean Sciences, St. Georges, Bermuda*
- TP 768 **Cellular dynamics of protein-protein interactions mediated by serine phosphorylation;** Kyle Mohler<sup>1</sup>; Karl Barber<sup>1</sup>; Jack Moen<sup>1</sup>; Svetlana Rogulina<sup>1</sup>; Jesse Rinehart<sup>1</sup>; <sup>1</sup>*Yale University, West Haven, CT*
- TP 772 **Investigating proteome changes caused by ABCA7 missense variants that confer Alzheimer's disease risk in African Americans;** Tyra M. Avery<sup>1</sup>; Kaitlyn E. Stepler<sup>1</sup>; Prem Prakash<sup>2</sup>; Jamaine S. Davis<sup>2</sup>; Renã A.S. Robinson<sup>1,3,4,5,6</sup>; <sup>1</sup>*Vanderbilt University Department of Chemistry, Nashville, TN;* <sup>2</sup>*Meharry Medical College Department of Biochemistry and Cancer Biology, Nashville, TN;* <sup>3</sup>*Vanderbilt University Medical Center Department of Neurology, Nashville, TN;* <sup>4</sup>*Vanderbilt Memory and Alzheimer's Center Vanderbilt University Medical Center, Nashville, TN;* <sup>5</sup>*Vanderbilt Institute of Chemical Biology, Nashville, TN;* <sup>6</sup>*Vanderbilt Brain Institute, Nashville, TN*
- TP 774 **Proteome-Wide Optimization of Orthogonal Translation Systems;** Jack M Moen<sup>1</sup>; Kyle Mohler<sup>1</sup>; Svetlana Rogulina<sup>1</sup>; Jesse Rinehart<sup>1</sup>; <sup>1</sup>*Yale University, West Haven, CT*
- WP 012 **The Eight(y) Million Pound Question: Using DESI Ambient MS Imaging for the Forensic Analysis of Cheque Fraud;** Huiqin Zhong<sup>1</sup>; Zhengwei Jia<sup>1</sup>; Wei Rao<sup>1</sup>; <sup>1</sup>*Waters Technologies?Shanghai?Co?Ltd, Shanghai, China*
- WP 029 **Intact metabolomics by PESI/MS/MS and its application to metabolic profiling of acetaminophen-induced acute hepatic injury model mice;** Tomomi Ohara<sup>1</sup>; Kenta Kondo<sup>1</sup>; Tasuku Murata<sup>2</sup>; Tetsuya Ishikawa<sup>3</sup>; Akira Ishii<sup>1</sup>; Hitoshi Tsuchihashi<sup>1</sup>; Koretsugu Ogata<sup>2</sup>; Yumi Hayashi<sup>3,4</sup>; Kei Zaito<sup>1,4</sup>; <sup>1</sup>*Department of Legal Medicine and Bioethics, Nagoya University Graduate School of Medicine, Nagoya, Japan;* <sup>2</sup>*Shimadzu Corporation, Kyoto, Japan;* <sup>3</sup>*Pathophysiological Laboratory Sciences, Department of Radiological and Medical Laboratory Sciences, Nagoya University Graduate School of Medicine, Nagoya, Japan;* <sup>4</sup>*In Vivo Real-Time Omics Laboratory, Institute for Advanced Research, Nagoya University, Nagoya, Japan*
- WP 034 **MS-based characterization of a novel antibody against Marburg virus nucleoprotein;** yanchun Lin<sup>1</sup>; Britney Johnson<sup>2</sup>; Angela Zou<sup>2</sup>; Kathleen C.F. Sheehan<sup>2</sup>; Gaya Amarasinghe<sup>2</sup>; Daisy Leung<sup>2</sup>; Michael L. Gross<sup>1</sup>; <sup>1</sup>*Department of Chemistry, Washington University in St Louis, St Louis, MO;* <sup>2</sup>*Department of Pathology and Immunology, Washington University School of Medicine, St Louis, MO*
- WP 041 **Enabling Single-cell Clone Selection for Knob-in-Hole Bispecific Antibodies via Automated Affinity Capture Coupled to High-throughput RapidFire Mass Spectrometry;** William Sawyer<sup>1</sup>; Neha Srikrumar<sup>2</sup>; Joseph Carver<sup>2</sup>; Phillip Y. Chu<sup>2</sup>; Amy Shen<sup>2</sup>; Ankai Xu<sup>2</sup>; Ambrose Williams<sup>2</sup>; Cong Wu<sup>2</sup>; Yichin Liu<sup>2</sup>; John C. Tran<sup>2</sup>; <sup>1</sup>*Genentech, South San Francisco, CA;* <sup>2</sup>*Genentech, Inc., South San Francisco, CA*
- WP 044 **A proteomic approach to single chain Camelid antibody discovery;** Anand Patel<sup>1</sup>; Natalie Castellana<sup>1</sup>; Thiago Lima<sup>1</sup>; Stefano Bonissone<sup>1</sup>; <sup>1</sup>*Digital Proteomics, LLC., San Diego, CA*
- WP 048 **Monitoring of DAR/ADC attributes for Trastuzumab Emtansine;** Sibylle Heidelberger<sup>1</sup>; Ferran Sanchez<sup>2</sup>; <sup>1</sup>*AB Sciex UK Ltd, Warrington, United Kingdom;* <sup>2</sup>*SCIEX, Madrid, Spain*
- WP 050 **Interactions of Hepatitis B Virus Capsids with Importin ? and Anti-viral Drugs Monitored by Charge Detection Mass Spectrometry;** Christine Kim<sup>1</sup>; Nicholas A. Lykтей<sup>1</sup>; Adam Zlotnick<sup>1</sup>; Martin F. Jarrold<sup>1</sup>; <sup>1</sup>*Indiana University, Bloomington, IN*



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- WP 052 **Characterization of N-Glycan species of VEGF decoy receptor fusion protein by novel HILIC-LC separation with high sensitive mass spectrometric characterization;** Mihir Mahendra Thakar<sup>1</sup>; Faraz Rasid<sup>2</sup>; Dipankar Malakar<sup>2</sup>; Bobby Virasingh<sup>1</sup>; Manoj Pillai<sup>2</sup>; <sup>1</sup>*Phenomenex India Pvt Ltd, Hyderabad, India*; <sup>2</sup>*SCIEX INDIA, GURUGRAM, India*
- WP 053 **Affinity purification of IdeZ digest for Glycosylation profile of Immunoglobulins using a linear benchtop MALDI-TOFMS;** Yuzo Yamazaki<sup>1</sup>; Shuichi Nakaya<sup>1</sup>; <sup>1</sup>*Shimadzu Corporation, Kyoto, Japan*
- WP 054 **Investigation of ocular tissue disposition of antibody-drug conjugates using novel LC-MS-based strategies;** Xiaoyu Zhu<sup>1</sup>; Ming Zhang<sup>2</sup>; Jie Pu<sup>1</sup>; Shihan Huo<sup>1</sup>; Chao Xue<sup>1</sup>; Jun Qu<sup>1,2</sup>; <sup>1</sup>*University at Buffalo, Buffalo, NY*; <sup>2</sup>*New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, New York*
- WP 056 **Optimization of a LC/MS Method for Disulfide Characterization and Free Cystine Quantification in Protein Therapeutics;** Song Nie<sup>1</sup>; Xin Chen<sup>1</sup>; Jun Lun<sup>1</sup>; <sup>1</sup>*Catalent Pharma Solutions, Madison, WI*
- WP 059 **High Resolution MS-based Structural Characterization Plays a Key Role in ADC Process Development;** Zhiqi Hao<sup>1</sup>; Diana Y. Liu<sup>1</sup>; Qiuting Hong<sup>2,3</sup>; Michael Kim<sup>1</sup>; William Haskins<sup>1,4</sup>; Tomasz Baginski<sup>1</sup>; Yan Chen<sup>1</sup>; <sup>1</sup>*Genentech, South San Francisco, CA*; <sup>2</sup>*Eurofins Lancaster Laboratories, Inc., Lancaster, PA*; <sup>3</sup>*Allakos Inc., Redwood City, CA*; <sup>4</sup>*Gryphon Bio Inc, South San Francisco, CA*
- WP 080 **Region-Specific N-Glycome Mapping of the Human Brain in Alzheimer's Patients by nanoLC chip-Q-TOF MS Analysis;** Jennyfer Tena<sup>1</sup>; Mariana Barboza<sup>1</sup>; Maurice Wong<sup>1</sup>; Carlito B Lebrilla<sup>1</sup>; <sup>1</sup>*University of California, Davis, Davis, CA*
- WP 084 **Phosphatidylcholines as a biomarker potential candidate of Multiple Sclerosis;** Fernando Brunale Leite<sup>1</sup>; Danielle Zildeana Furtado<sup>1</sup>; Cleber Nunes Barreto<sup>1</sup>; Erica Souza Silva<sup>1</sup>; Nilson Antonio Assuncao<sup>1</sup>; <sup>1</sup>*Unifesp, São Paulo, Brazil*
- WP 085 **Proteome and phosphoproteome biomarker discovery strategies for biopsy-free bladder cancer diagnosis based on urinary extracellular vesicles;** Xiaofeng Wu<sup>1</sup>; Sebastian Paez<sup>1</sup>; Hristos Kaimakliotis<sup>2</sup>; Anton B. Iliuk<sup>3</sup>; Weiguo Andy Tao<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*Indiana University School of Medicine, Indianapolis, Indiana*; <sup>3</sup>*Tymora Analytical Operations, West Lafayette, IN*
- WP 087 **Deciphering Racial Disparities in Breast Cancer by Novel Extracellular Matrix Proteomic Approaches on Formalin-Fixed, Paraffin-Embedded Clinical Specimens;** Peggy M. Angel<sup>1</sup>; Baylye Boxall<sup>1</sup>; Jennifer R. Bethard<sup>1</sup>; Lauren E. Ball<sup>1</sup>; Jeffrey R. Marks<sup>2</sup>; Richard R. Drake<sup>1</sup>; <sup>1</sup>*Medical University of South Carolina, Charleston, SC*; <sup>2</sup>*Duke University School of Medicine, Durham, NC*
- WP 091 **UTiDx: 60 second assay for detecting urinary tract infections;** Dominique G Bihan<sup>1</sup>; Spencer D Wildman<sup>1</sup>; Daniel B Gregson<sup>2</sup>; Thomas Rydzak<sup>1</sup>; Ryan A Groves<sup>1</sup>; Carly Y Chan<sup>1</sup>; Deirdre L Church<sup>2</sup>; Ian A Lewis<sup>1</sup>; <sup>1</sup>*University of Calgary, Calgary, AB*; <sup>2</sup>*Calgary Laboratory Services, Alberta Health Services, Calgary, AB*
- WP 100 **IDENTIFICATION CLOSTRIDIUM CHAUVOEI BY MALDI-TOF MS FROM PARAFFIN EMBEDDED SECTIONS OF LOWER EXTREMITY INFECTIONS, IN THREE DIABETES PATIENTS AFTER AMPUTATIONS;** Barbara Dominiak<sup>1</sup>; Maria Anita Mendes<sup>2,3,4,5</sup>; <sup>1</sup>*Temple University, Philadelphia, PA*; <sup>2</sup>*Dampster Mass Spectrometry Lab, Sao Paulo-SP,, Brazil*; <sup>3</sup>*William Oxberry, Brooklyn, New York, SUNY Downstate Medical Center*; <sup>4</sup>*Patrick Chen, Brooklyn, SUNY Downstate Medical Center, New York*; <sup>5</sup>*Ernieque ER Sanches, Dampster Mass Spectrometry Lab., Brazil*
- WP 106 **Utilizing Blood Cards for Quantitative Assessment of Glutathione as an Important Biomarker Test for Autism Spectrum Disorder and Neurodegenerative Diseases;** Ashley Trouten<sup>1</sup>; H. m. Skip Kingston<sup>1</sup>; <sup>1</sup>*Duquesne University, Pittsburgh, PA*
- WP 120 **Post-translationally modified proteins in plasma extracellular vesicles as candidate markers for breast cancer subtypes;** Hillary Andaluz Aguilar<sup>1</sup>; I-Hsuan Chen<sup>1</sup>; J. Sebastian Paez<sup>1</sup>; Anton B. Iliuk<sup>2</sup>; Sonia Sugg<sup>3</sup>; Weizhou Zhang<sup>3</sup>; Weiguo Andy Tao<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*Tymora Analytical Operations, West Lafayette, IN*; <sup>3</sup>*University of Iowa, Iowa City, Iowa*





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- WP 134 **Monitoring of hSCN binding-site using Multiple MS-based Methods;** Chunyang Guo<sup>1</sup>; Lindsey Steinberg<sup>2</sup>; Ming Cheng<sup>1</sup>; Jing Yan<sup>1</sup>; Jeffrey P Henderson<sup>2</sup>; Michael L Gross<sup>1</sup>; <sup>1</sup>*Department of Chemistry, Washington University in St Louis, St Louis, MO*; <sup>2</sup>*Division of Infectious Diseases, Department of Medicine, Washington University School of Medicine, St Louis, Missouri*
- WP 140 **Sub-residue Resolution Footprinting of Ligand-Protein Interactions Enabled by Ion Mobility Mass Spectrometry;** Gaoyuan Lu<sup>1</sup>; Nian Wang<sup>1</sup>; Yang Tian<sup>1</sup>; Ning Wan<sup>1</sup>; Yatao Shi<sup>2</sup>; Gongyu Li<sup>2</sup>; Lingjun Li<sup>2</sup>; Haiping Hao<sup>1</sup>; Hui Ye<sup>1</sup>; <sup>1</sup>*China Pharmaceutical University, Nanjing, Jiangsu, China*; <sup>2</sup>*University of Wisconsin - Madison, madison*
- WP 142 **Mechanistic studies of radical trifluoromethylation and its application for membrane protein labeling and epitope mapping;** Ming Cheng<sup>1</sup>; Chunyang Guo<sup>1</sup>; George Mathai<sup>2</sup>; Gary Gerstenecker<sup>1</sup>; Don Rempel<sup>1</sup>; Michael L. Gross<sup>1</sup>; <sup>1</sup>*Washington University, St.louis, MO*; <sup>2</sup>*Sacred Heart College, Cochin, India*
- WP 146 **Mass spectrometry-based protein footprinting reveals conformational dynamics of the plasma membrane proton pump;** Thao T. Nguyen<sup>1</sup>; Pei Liu<sup>2</sup>; Benjamin Minkoff<sup>1</sup>; Michael Sussman<sup>1</sup>; <sup>1</sup>*UW Madison, Madison, WI*; <sup>2</sup>*University of Missouri, Columbia, MO*
- WP 158 **Rapid Multiplexed Analysis of Cannabinoids and their Metabolites in Urine using MassHunter StreamSelect LC-MS System;** Andre Szczesniewski<sup>1</sup>; Kevin McCann<sup>1</sup>; <sup>1</sup>*Agilent Technologies, Wood Dale, IL*
- WP 160 **Quantitation of California Regulated Pesticides in Cannabis Oil by ESI/APCI UHPLC-MS-MS;** Jacob Jalali<sup>1</sup>; Avinash Dalmia<sup>2</sup>; Erasmus Cudjoe<sup>3</sup>; Feng Qin<sup>3</sup>; Jingcun wu<sup>3</sup>; Luke Ward<sup>4</sup>; Ben Armstrong<sup>4</sup>; <sup>1</sup>*PerkinElmer, San Jose, CA*; <sup>2</sup>*PerkinElmer, Shelton, CT*; <sup>3</sup>*PerkinElmer, Woodbridge, ON*; <sup>4</sup>*Juniper Analytics, Bend, OR*
- WP 161 **Similarities and differences in the fragmentation pathways of cannabinoid ions generated by electron impact, electrospray ionization, atmospheric pressure chemical ionization;** Allegra Leghissa<sup>1</sup>; Zacariah L. Hildenbrand<sup>2</sup>; Kevin A Schug<sup>3</sup>; <sup>1</sup>*University of Texas, Arlington, Arlington, TX*; <sup>2</sup>*Inform Environmental LLC., Dallas, Texas*; <sup>3</sup>*University of Texas Arlington, Arlington*
- WP 162 **A Draft Map of the Cannabis Proteome;** Benjamin Orsburn<sup>1</sup>; Conor Jenkins<sup>1,2</sup>; <sup>1</sup>*Think20 Labs, Columbia, MD*; <sup>2</sup>*Hood College Bioinformatics Program, Frederick, MD*
- WP 167 **Does Your Dog Have Anxiety After a Rough Day at the Lake: Analysis of CBD Extracts for Dog Treats;** Matthew Curtis<sup>1</sup>; Mike Adams<sup>2</sup>; Karen Kaikaris<sup>2</sup>; Sarah Aijaz<sup>3</sup>; Sue D'Antonio<sup>1</sup>; Anthony Macherone<sup>1,4</sup>; <sup>1</sup>*Agilent Technologies, Inc., Santa Clara, CA*; <sup>2</sup>*CWC Labs, Cedar Creek, TX*; <sup>3</sup>*MilliporeSigma, Bellefonte, PA*; <sup>4</sup>*Johns Hopkins University School of Medicine, Baltimore, MD*
- WP 168 **Time saving sample prep for the analysis of 54 residues in cannabis flower by LC-MS/MS;** Lisa Wanders; *Thomson Instrument Co, Oceanside, CA*
- WP 170 **An Automated LC-MS/MS Workflow for High-throughput Pesticide Residue Screening in Cannabis Samples;** Mahsan Miladi<sup>1</sup>; Tanner Stevenson<sup>1</sup>; <sup>1</sup>*Agilent Technologies, Santa Clara, CA*
- WP 173 **Screening CBD Oil Pet Supplements for Mycotoxins using LC-MS Quadrupole System with Accurate Mass Calibration;** Sue D'Antonio<sup>1</sup>; Yongdong Wang<sup>2</sup>; Don Kuehl<sup>2</sup>; Anthony Macherone<sup>3,4</sup>; <sup>1</sup>*Agilent Technologies, Inc., Santa Clara, CA*; <sup>2</sup>*Cerno Bioscience LLC, Norwalk, CT*; <sup>3</sup>*Agilent Technologies, Wilmington, DE*; <sup>4</sup>*Johns Hopkins University School of Medicine, Baltimore, MD*
- WP 196 **Investigation on isomeric gangliosides using LC/MS/MS towards mouse brain regional mapping;** Jua Lee<sup>1</sup>; Jaekyung Yun<sup>1</sup>; Heeyoun Hwang<sup>1</sup>; Hee-sup Shin<sup>2</sup>; Hyun Joo An<sup>1</sup>; <sup>1</sup>*Chungnam National University, Daejeon, South Korea*; <sup>2</sup>*Institute for basic science, Daejeon, South Korea*
- WP 207 **An ultra-sensitive paper-based diagnostic platform of detecting colorectal cancer via mass spectrometry;** Suji Lee<sup>1</sup>; Abraham K. Badu-Tawiah<sup>1</sup>; <sup>1</sup>*The Ohio State University, Columbus, OH*
- WP 208 **Rapid, robust and high-throughput proteome analysis by high-flow LC-MS/MS;** Yangyang Bian<sup>1</sup>; Runsheng Zheng<sup>1</sup>; Yun-Chien Chang<sup>1</sup>; Jana Zecha<sup>1</sup>; Stephanie Heinzlmeir<sup>1</sup>; Daniel P Zolg<sup>1</sup>; Oleksandr



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- Boichenko<sup>2</sup>; Mike Baynham<sup>3</sup>; Bernhard Kuster<sup>1,4,5</sup>; <sup>1</sup>*Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany*; <sup>2</sup>*Thermo Fisher Scientific, Germering, Germany*; <sup>3</sup>*Thermo Fisher Scientific, Runcorn, United Kingdom*; <sup>4</sup>*Center for Integrated Protein Science Munich, Freising, Germany*; <sup>5</sup>*Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany*
- WP 209 **A High Throughput and High Resolution LC-MS/MS Method to Measure IGF1 in Serum for Clinical Research;** Xiaolei Xie; *ThermoFisher Scientific, San Jose, CA*
- WP 215 **Application of the HPLC-MS/MS method in studying individual metabolic differences of cyclosporin A in bone marrow transplant patients;** Wang Lei<sup>1,2</sup>; Liu hong xing<sup>2,3,4</sup>; Liu rui<sup>1</sup>; Yang zi yi<sup>1</sup>; <sup>1</sup>*HebeiYanda Lu Daopei Hospital, Langfang, China*; <sup>2</sup>*Beijing Lu Daopei Hospital, Beijing, China*; <sup>3</sup>*HebeiYanda Lu Daopei Hospita, Langfang, China*; <sup>4</sup>*Beijing Lu Daopei Institute of Hematology, Beijing, China*
- WP 218 **Reliable Quantification of 52 Amino Acids in Human Plasma by LC-MS/MS;** Stephanie Samra<sup>1</sup>; Valérie Thibert<sup>2</sup>; Claude Netter<sup>2</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*Thermo Fisher Scientific, Courtaboeuf, France*
- WP 219 **High-Sensitivity Analysis of a Steroid Panel Samples using Micro-Flow LC-MS/MS for Clinical Research;** Narumi Shirai<sup>1</sup>; Takanari Hattori<sup>2</sup>; Mikael Levi<sup>2</sup>; Shoji F. Nakayama<sup>3</sup>; Shigeru Suzuki<sup>1</sup>; <sup>1</sup>*Chubu University, Kasugai, Japan*; <sup>2</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>3</sup>*National Institute for Environmental Studies, Tsukuba, Japan*
- WP 220 **Using Superficially Porous Phenyl Phase Selectivity for Benzodiazepine Separations;** William Long<sup>1</sup>; Carl Griffin<sup>2</sup>; Anne E Mack<sup>2</sup>; Emily Parry<sup>2</sup>; Charles Lofton<sup>2</sup>; <sup>1</sup>*Agilent Technologies, Wilmington, DE*; <sup>2</sup>*Agilent Technologies, Inc., Wilmington, DE*
- WP 224 **Case-Control Study: Expanded proteomics and lipidomic profiling for early prediction of major adverse cardiac events;** Qin Fu<sup>1</sup>; Irina Tchernyshyov<sup>1</sup>; Ronald Holewinski<sup>1</sup>; Vidya Venkatraman<sup>1</sup>; David Sarracino<sup>2</sup>; Casey Johnson<sup>1</sup>; Kelly Njine Mouapi<sup>1</sup>; Susan Cheng<sup>3</sup>; Chrisandra Shufelt<sup>3</sup>; Brennan Spiegel<sup>4</sup>; Noel Bairey Merz<sup>3</sup>; Scott Peterman<sup>2</sup>; Jennifer Van Eyk<sup>1,3</sup>; <sup>1</sup>*Advanced Clinical Biosystems Research Institute, The Smidt Heart Institute, Cedars-Sinai Medical Center, Los Angeles, CA 90048, Los Angeles,, CA*; <sup>2</sup>*Thermo Fisher Scientific, Cambridge, MA*; <sup>3</sup>*Barbra Streisand Women's Heart Center, The Smidt Heart Institute, Cedars-Sinai Medical Center, Los Angeles, CA*; <sup>4</sup>*Clinical and Translational Science Institute, Cedars-Sinai Medical Center, Los Angeles, CA*
- WP 227 **Ambient mass spectrometry mapping of lipid fingerprints in healthy and cancerous human colorectal tissues;** Yasmin Shanneik<sup>1</sup>; Emrys A. Jones<sup>2</sup>; Bipasha Chakrabarty<sup>3</sup>; Kaye J. Williams<sup>4</sup>; Omer Aziz<sup>3</sup>; Steven Pringle<sup>2</sup>; Adam W. McMahon<sup>1</sup>; <sup>1</sup>*Wolfson molecular imaging centre, The University of manchester, Manchester, United Kingdom*; <sup>2</sup>*Waters Corporation, Manchester, United Kingdom*; <sup>3</sup>*The Christie NHS Foundation Trust, Manchester, United Kingdom*; <sup>4</sup>*The University of Manchester, Division of Pharmacy & Optometry, Manchester, United Kingdom*
- WP 233 **Quantitative proteomic assessment of differences and stability of human serum and plasma proteins;** Sumio Ohtsuki<sup>1</sup>; Madoka Nanbu<sup>1</sup>; Shin Nishiumi<sup>2</sup>; Takashi Kobayashi<sup>2</sup>; Shingo Ito<sup>1</sup>; Takeshi Masuda<sup>1</sup>; Masaru Yoshida<sup>2</sup>; <sup>1</sup>*Kumamoto University, Kumamoto, Japan*; <sup>2</sup>*Kobe University, Kobe, Japan*
- WP 235 **Label-free drug discovery with mass spectrometry: high-throughput screening of enzyme modulators as anticancer candidates;** Alireza Abdolvahabi<sup>1</sup>; John J. Bowling<sup>1</sup>; Duane G. Currier<sup>1</sup>; Zoran Rankovic<sup>1</sup>; <sup>1</sup>*St Jude Children's Research Hospital, Memphis, TN*
- WP 236 **Drug Discovery Applications of ADE-OPP-MS (Acoustic-Droplet-Ejection coupled Open-Port-Probe Mass Spectrometry) Platform;** Hui Zhang<sup>1</sup>; Wenyi Hua<sup>1</sup>; Chang Liu<sup>2</sup>; Jianua Liu<sup>1</sup>; David Cox<sup>2</sup>; Anthony Carlo<sup>1</sup>; Matt Troutman<sup>1</sup>; Tom Covey<sup>2</sup>; <sup>1</sup>*Pfizer Inc., Groton, CT*; <sup>2</sup>*SCIEX, Concord, ON*
- WP 245 **High Resolution MS for 3D Culture Hepatic In Vitro Models Metabolite Identification;** Sujoy Lahiri<sup>1</sup>; Kate Comstock<sup>2</sup>; <sup>1</sup>*Thermo Fisher Scientific, Frederick, MD*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*



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- WP 248 **Stereoisomer Separation of Drugs and Biomarkers Using Supercritical Fluid Chromatography to Support PK/PD Studies;** Fangbiao Li<sup>1</sup>; Bang-lin Wan<sup>2</sup>; Guangping Bi<sup>2</sup>; Rena Zhang<sup>2</sup>; Daniel Spellman<sup>2</sup>; <sup>1</sup>Merck & Co., Inc., West Point, PA; <sup>2</sup>Merck & Co., Inc., West Point, PA
- WP 249 **LC-MS for bioanalysis of a wide range of biotherapeutic modalities;** Hao Jiang<sup>1</sup>; Alex Kozhich<sup>1</sup>; Linlin Luo<sup>1</sup>; Wendy Miller<sup>1</sup>; Craig Titsch<sup>1</sup>; Johanna Mora<sup>1</sup>; Gerry Kolaitis<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb, Princeton, NJ
- WP 250 **Ion Mobility-Enabled Metabolite Identification of Tienilic Acid and Tienilic Acid Isomer;** Lauren Mullin<sup>1</sup>; Giorgis Isaac<sup>1</sup>; Ian D Wilson<sup>2</sup>; Gordon Murray<sup>3</sup>; Nathan Andersen<sup>1</sup>; Robert S Plumb<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Imperial College London, London, SW7 2AZ; <sup>3</sup>Waters Corp., Beverly, MA
- WP 262 **Phytochemicals and their metabolites as the exposure biomarkers of whole grain intake;** Shengmin Sang<sup>1</sup>; Yingdong Zhu<sup>1</sup>; Pei Wang<sup>1</sup>; Shuwei Zhang<sup>1</sup>; Yao Tang<sup>1</sup>; <sup>1</sup>North Carolina A&T State University, Kannapolis, NC
- WP 263 **Rapid-Throughput Characterization of Dietary Fiber Supplements Employing UHPLC/QqQ MS;** Thai-thanh T Vo<sup>1</sup>; Matthew J. Amicucci<sup>2</sup>; Eshani Nandita<sup>2</sup>; Ace G. Galermo<sup>1</sup>; Megan A. Lee<sup>2</sup>; Yiyun Liu<sup>2</sup>; Carlito B. Lebrilla<sup>2</sup>; <sup>1</sup>University of California Davis, Davis, CA; <sup>2</sup>University of California, Davis, Davis, CA
- WP 274 **In-depth Profiling of Beetroot Bioactive Compounds by DAD-ESI-LC/MS/MS;** Nebiyu Abshiru<sup>1</sup>; Boris Nemzer<sup>1</sup>; <sup>1</sup>VDF FutureCeuticals, Inc, Momence, IL
- WP 279 **High-throughput online micro-SPE with LCMS/MS analysis of multiple pesticides residues in fruits and vegetables;** Jianzhong Li<sup>1</sup>; Ye Kong<sup>1</sup>; Zhe Cao<sup>1</sup>; <sup>1</sup>No.3, Wang Jing Bei Lu, Beijing, China
- WP 288 **Determination of Glyphosate in Animal Feed Matrices by QuPPE Extraction and LC-MS/MS Detection;** Joanne L Baillie<sup>1</sup>; Fang Shi<sup>1</sup>; <sup>1</sup>Canadian Food Inspection Agency, Calgary, AB
- WP 301 **Off-Line Hydrogen Cleaning of GC/MS Ion Source Increases Sample Throughput for Pesticides in Foods;** Jochen Stoeppler<sup>1</sup>; Joerg Riener<sup>2</sup>; Klaus Wilmers<sup>1</sup>; Thorsten Bernsmann<sup>1</sup>; Courtney Milner<sup>3</sup>; <sup>1</sup>Chemisches und Veterinäruntersuchungsamt Münsterland-Emscher-Lippe (CVUA-MEL), Muenster, Germany; <sup>2</sup>Agilent Technologies, Waldbronn, Germany; <sup>3</sup>Agilent, Santa Clara, CA
- WP 302 **Is washing and/or cooking of vegetables enough to minimize the risk of population exposure to pesticide residues?;** Joshua Ye<sup>1</sup>; Jingcun Wu<sup>2</sup>; Erasmus Cudjoe<sup>2</sup>; Feng Qin<sup>2</sup>; <sup>1</sup>PerkinElmer Inc., Woodbridge, ON; <sup>2</sup>PerkinElmer, Inc., Woodbridge, ON
- WP 304 **Reduction of disulfide bonds using a high-powered femtosecond laser;** Simon K. Gammelgaard<sup>1, 2</sup>; Steffen B. Petersen<sup>2</sup>; Kim F. Haselmann<sup>1</sup>; Peter Kresten Nielsen<sup>1</sup>; <sup>1</sup>Novo Nordisk A/S, Måløv, Denmark; <sup>2</sup>Aalborg University, Aalborg, Denmark
- WP 309 **Rapid "Shotgun" APGC-Ion Mobility Mass Spectrometry for the Analysis of Phytosterols in Honey Bee Dietary Pollen;** Jeffrey T Morre<sup>1</sup>; Priyadarshini Chakrabarti<sup>1</sup>; Diana Oppenheimer<sup>1</sup>; Ramesh R Sagili<sup>1</sup>; Claudia S. Maier<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, OR
- WP 321 **DMEITM source with a reaction cell - A new advances in ion generation for GC-MS/MS;** Harikrishnan Sukumar<sup>1</sup>; Heather Gamble<sup>1</sup>; Dante Sanchez<sup>1</sup>; Victor Titov<sup>1</sup>; Anna Kornilova<sup>1</sup>; Reza Javahery<sup>1</sup>; <sup>1</sup>PerkinElmer Inc., Woodbridge, ON
- WP 332 **Analysis of Mucin Proteins by Charge Detection Mass Spectrometry;** Lauren F Barnes<sup>1</sup>; Benjamin E Draper<sup>1</sup>; Nicholas A Lykтей<sup>1</sup>; Martin F Jarrold<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN
- WP 336 **Modification of Cell Membrane Glycosylation with Inhibitors and Characterization with nanoLC-MS;** Qing W Zhou<sup>1</sup>; Yixuan Xie<sup>2</sup>; Qiongyu Li<sup>1</sup>; Maurice Wong<sup>3</sup>; Carlito B Lebrilla<sup>1</sup>; <sup>1</sup>University of California, Davis, Davis, CA; <sup>2</sup>Univerisity of California, Davis, Davis, CA; <sup>3</sup>University of California Davis, Davis, CA
- WP 340 **Identification of N-glycopeptides using Electron Transfer/High-energy Collision Dissociation (ETHcD);** Rui Zhang<sup>1</sup>; Xue Dong<sup>2</sup>; Jianhui Zhu<sup>3</sup>; David M. Lubman<sup>3</sup>; Yehia Mechref<sup>2</sup>; Haixu Tang<sup>1</sup>; <sup>1</sup>Indiana University Bloomington, Bloomington, IN; <sup>2</sup>Texas Tech University, Lubbock, TX; <sup>3</sup>University of Michigan Medical Center, Ann Arbor, MI



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- WP 342 **Characterizing HIV-1 Envelope N-glycan Shield: A Glycomics and Bioinformatics Method;** Audra Hargett<sup>1</sup>; Qing Wei<sup>1</sup>; Barbora Knoppova<sup>2</sup>; Stacy Hall<sup>1</sup>; Milan Raska<sup>1,2</sup>; Zina Moldoveanu<sup>1</sup>; Todd Green<sup>1</sup>; Jan Novak<sup>1</sup>; Matthew B. Renfrow<sup>1</sup>; <sup>1</sup>*University of Alabama at Birmingham, Birmingham, AL*; <sup>2</sup>*Palacky University in Olomouc, Olomouc, Czech Republic*
- WP 348 **Determination of Human Immunoglobulin Glycoforms by timsTOF Pro Sequencing Analysis;** Kim Alving<sup>1</sup>; Anjali Alving<sup>2</sup>; Aharon Cohen<sup>1</sup>; Bing Wang<sup>1</sup>; <sup>1</sup>*Sanofi, Waltham, MA*; <sup>2</sup>*Bruker Scientific, Billerica, MA*
- WP 349 **Fast analysis of glycans using LC-MS and Proteinase K Digestion;** Suping Zheng<sup>1</sup>; Jie Ding<sup>1</sup>; <sup>1</sup>*PPD, Inc., Middleton, WI*
- WP 373 **Reproducibility of MALDI Imaging Based Tissue Classifications - Results of a Multi-Center Study;** Soeren-oliver Deininger<sup>1</sup>; Rita Casadonte<sup>2</sup>; Petra Wandernoth<sup>2</sup>; Kristina Schwamborn<sup>3</sup>; Christine Bollwein<sup>3</sup>; Christian Marsching<sup>4</sup>; Katharina Kriegsmann<sup>5</sup>; Carsten Hopf<sup>4</sup>; Wilko Weichert<sup>3</sup>; Jörg Kriegsmann<sup>2</sup>; Peter Schirmacher<sup>6</sup>; Mark Kriegsmann<sup>6</sup>; Alice Ly<sup>1</sup>; <sup>1</sup>*Bruker Daltonik GmbH, Bremen, Germany*; <sup>2</sup>*Proteopath, Trier, Germany*; <sup>3</sup>*Institute of Pathology, Technical University of Munich, Munich, Germany*; <sup>4</sup>*Center for Biomedical Mass Spectrometry and Optical Spectroscopy (CeMOS), Mannheim University of Applied Sciences, Mannheim, Germany*; <sup>5</sup>*Department of Hematology, Oncology and Rheumatology, University Hospital Heidelberg, Heidelberg, Germany*; <sup>6</sup>*Institute of Pathology, University Hospital Heidelberg, Heidelberg, Germany*
- WP 375 **Spatial Information of Metabolites Using Mass Spectrometry Imaging on Breast Needle Biopsy Using DEFFI-MS;** Vincen Wu<sup>1</sup>; Paolo Inglese<sup>2</sup>; Hui-Yu Ho<sup>2</sup>; Andreas Dannhorn<sup>3</sup>; Emine Kazanc<sup>2</sup>; Goncalo Correia<sup>2</sup>; James Mckenzie<sup>2</sup>; Stephanie Ling<sup>3</sup>; Evdoxia Karali<sup>4</sup>; Nikolaos Koundouros<sup>4</sup>; Hiromi Kudo<sup>2</sup>; Peter Kreuzaler<sup>5</sup>; Sami Shousha<sup>2</sup>; Ian Gilmore<sup>6</sup>; Mariia Yuneva<sup>5</sup>; Richard Goodwin<sup>3</sup>; Josephine Bunch<sup>6</sup>; George Poulogiannis<sup>4</sup>; Zoltan Takats<sup>2</sup>; <sup>1</sup>*Imperial College London, London, United Kingdom*; <sup>2</sup>*Imperial College, London, United Kingdom*; <sup>3</sup>*AstraZeneca, iMED, United Kingdom*; <sup>4</sup>*Institute of Cancer Research, London, United Kingdom*; <sup>5</sup>*Francis Crick Institute, London, United Kingdom*; <sup>6</sup>*National Physical Laboratory, London, United Kingdom*
- WP 379 **A novel strategy for the pathological study of Alzheimer's Disease brain with MALDI Imaging Mass Spectrometry with shotgun proteomics;** Masaya Ikegawa<sup>1</sup>; Nobuto Kakuda<sup>1</sup>; Tomohiro Miyasaka<sup>1</sup>; Takashi Nirasawa<sup>2</sup>; Ryo Kajita<sup>2</sup>; Shigeo Murayama<sup>3</sup>; Yasuo Ihara<sup>4</sup>; <sup>1</sup>*Doshisha university, Kyotanabe City, Japan*; <sup>2</sup>*Bruker Japan K.K., Yokohama, Japan*; <sup>3</sup>*The Brain Bank for Aging Research, Tokyo Metropolitan Geriatric Hospital and Institute of Gerontology, Tokyo, Japan*; <sup>4</sup>*Graduate School of Brain Science, Doshisha University, Kyotanabe City, Japan*
- WP 380 **A Ground Truth MS1 Data Set for Quantitative Evaluation of Precursor-Aware Proteomics Mass Spectrometry Data Processing Algorithms;** Jessica Henning<sup>1</sup>; Annika Tostengard<sup>1</sup>; Robert Smith<sup>1</sup>; <sup>1</sup>*University of Montana, Missoula, MT*
- WP 383 **MIND: A double-linear model to accurately determine monoisotopic precursor mass in high-resolution top-down proteomics;** Frederik Lermyte<sup>1</sup>; Piotr Dittwald<sup>2</sup>; Jürgen Claesen<sup>3</sup>; Geert Baggerman<sup>4</sup>; Frank Sobott<sup>5</sup>; Peter B. O'Connor<sup>1</sup>; Kris Laukens<sup>4</sup>; Jef Hooyberghs<sup>6</sup>; Anna Gambin<sup>2</sup>; Dirk Valkenborg<sup>3</sup>; <sup>1</sup>*University of Warwick, Coventry, United Kingdom*; <sup>2</sup>*University of Warsaw, Warsaw, Poland*; <sup>3</sup>*Hasselt University, Hasselt, Belgium*; <sup>4</sup>*University Of Antwerp, Antwerp, Belgium*; <sup>5</sup>*University of Leeds, Leeds, United Kingdom*; <sup>6</sup>*Flemish Institute for Technological Research (VITO), Mol, Belgium*
- WP 387 **Identification of alternative-splicing events present in proteins using mass spectrometry and a custom sequence database of junction-spanned peptides;** Bang-Jie Han<sup>1</sup>; Pang-Hung Hsu<sup>1</sup>; Wen-Shyong Tzou<sup>1</sup>; <sup>1</sup>*National Taiwan Ocean University, Keelung, Taiwan*
- WP 388 **Tree based machine learning methods improve error rates in quality control of mass spectrometry-based proteomics;** Eralp Dogu<sup>1</sup>; Shantam Gupta<sup>2</sup>; Roger Olivella<sup>3</sup>; Eduard Sabido<sup>3</sup>; Olga Vitek<sup>4</sup>; <sup>1</sup>*Mugla*



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- University, Mugla, Turkey; <sup>2</sup>Quantiphi Inc, Boston, Massachusetts; <sup>3</sup>CRG, Barcelona, Spain; <sup>4</sup>Northeastern University, Boston, MA
- WP 389 **Deep learning methods applied to the analysis of metabolomics data;** Shinji Kanazawa<sup>1,2,3</sup>; Yohei Yamada<sup>1</sup>; Hiroyuki Yasuda<sup>1</sup>; Akihiro Kunisawa<sup>1</sup>; Toru Shiohama<sup>1</sup>; Shigeki Kajihara<sup>1</sup>; Norio Mukai<sup>1</sup>; Masaki Kakisako<sup>4</sup>; Go Fujisawa<sup>4</sup>; Yuzuru Yamakage<sup>4</sup>; Junko Iida<sup>1,2</sup>; Eiichiro Fukusaki<sup>5</sup>; Fumio Matsuda<sup>3</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>Osaka University Shimadzu Analytical Innovation Research Laboratory, Osaka University, Osaka, Japan; <sup>3</sup>Graduate School of Information Science and Technology, Osaka University, Osaka, Japan; <sup>4</sup>Fujitsu Limited, Tokyo, Japan; <sup>5</sup>Graduate School of Engineering, Osaka University, Osaka, Japan
- WP 402 **A Novel Data-Adaptive Robust Method for Quantifying Tissue Specificity Scores;** Meng Wang<sup>1</sup>; Lihua Jiang<sup>2</sup>; Hua Tang<sup>2</sup>; Michael Snyder<sup>2</sup>; <sup>1</sup>Stanford University, Stanford; <sup>2</sup>Stanford University, Palo Alto, CA
- WP 413 **Feature-Based Molecular Networking of Untargeted Mass Spectrometry Data: Bridging MS-DIAL, MZmine2, MetaboScape, OpenMS, and XC-MS, with the GNPS web-platform;** Louis Felix Nothias<sup>1</sup>; Daniel Petras<sup>1</sup>; Mingxun Wang<sup>1</sup>; Robin Schmid<sup>1,2</sup>; Abinesh Sarvepalli<sup>1</sup>; Zheng Zhang<sup>1</sup>; Ricardo da Silva<sup>1</sup>; Pieter Dorrestein<sup>1</sup>; <sup>1</sup>University of California, San Diego, La Jolla, CA; <sup>2</sup>University of Muenster, Institute of Inorganic and Analytical Chemistry, Muenster, Germany
- WP 414 **Deuterater: An Analyte-Agnostic Refactoring of Kinetic Analysis Software for Deuterium-Labeled Metabolomics;** Kyle J Cutler<sup>1</sup>; Russell Denton<sup>1</sup>; John C Price<sup>1</sup>; <sup>1</sup>Brigham Young University, Provo, UT
- WP 421 **MetGem Software for the Generation of Molecular Networks Based on the t-SNE Algorithm;** Nicolas Elie<sup>1</sup>; Florent Olivon<sup>1</sup>; Gwendal Grelier<sup>1</sup>; Fanny Roussi<sup>1</sup>; Marc Litaudon<sup>1</sup>; David Touboul<sup>1</sup>; <sup>1</sup>CNRS-ICSN, Gif-Sur-Yvette, France
- WP 427 **Uniting metabolomics data processing and highly confident annotation across six MS instrumental set ups: MetaboScape 5.0;** Nikolas Kessler<sup>1</sup>; Wiebke Timm<sup>1</sup>; Sascha Winter<sup>1</sup>; Ulrike Schweiger-Hufnagel<sup>1</sup>; Sven W. Meyer<sup>1</sup>; Aiko Barsch<sup>1</sup>; Heiko Neuweiger<sup>1</sup>; <sup>1</sup>Bruker Daltonics, Bremen, Germany
- WP 428 **Retention Time Prediction of Dansyl Labeled Tripeptides Using Machine Learning Methods for Dansylation LC-MS Metabolomics;** Hao Li<sup>1</sup>; Liang Li<sup>2</sup>; <sup>1</sup>University of Alberta, Edmonton; <sup>2</sup>University of Alberta, Edmonton, AB
- WP 436 **Performance evaluation of a modified Quadropole Orbitrap mass spectrometer;** Tabiwang N. Arrey<sup>1</sup>; Rosa Jersie-Christensen Rakownikow<sup>1</sup>; Julia Kraegenbring<sup>1</sup>; Kerstin Strupat<sup>1</sup>; Markus Kellmann<sup>1</sup>; Catharina Crone<sup>1</sup>; Thomas Moehring<sup>1</sup>; Alexander Harder<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Bremen, Germany
- WP 474 **Improved Integration of a Separation Column to an Ion Source for Liquid Chromatography Mass Spectrometry;** Michael Fogwill<sup>1</sup>; Angela Doneanu<sup>1</sup>; Stephen Hattan<sup>1</sup>; Jason Hill<sup>1</sup>; Wade P Leveille<sup>1</sup>; Thomas McDonald<sup>1</sup>; Joseph Michienzi<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA
- WP 476 **Advanced analytics for regulatory science: Application of an innovative robotic sample separation system coupled with tandem mass spectrometry;** Jinhui Zhang<sup>1</sup>; Patrick J. Faustino<sup>1</sup>; <sup>1</sup>FDA, Silver Spring, MD
- WP 477 **Growing MS adoption: A "Self-Driving" Mass Spectrometer Designed for Non-MS Experts;** Maggie A. Ostrowski<sup>1</sup>; F. Robert Ley<sup>1</sup>; Kyle Covert<sup>1</sup>; Kai Zhang<sup>1</sup>; Susan Shen<sup>1</sup>; Shane E. Tichy<sup>1</sup>; <sup>1</sup>Agilent Technologies, Inc., Santa Clara, CA
- WP 480 **Use of DESI with IMS enhancement in study of transferred material on paper;** Liepin Huang<sup>1</sup>; Carrie L Hogue<sup>2</sup>; Gilbert Castillo<sup>2</sup>; <sup>1</sup>Corning Inc., Horseheads, NY; <sup>2</sup>Corning Inc., Painted Post, 14870
- WP 481 **Collision induced unfolding experiments to decipher the structural regions of a hybrid monoclonal antibody.;** Thomas Botzanowski<sup>1</sup>; Oscar Hernandez-Alba<sup>1</sup>; Olivier Colas<sup>2</sup>; Elsa Wagner-Rousset<sup>2</sup>; Alain Beck<sup>2</sup>; Sarah Cianferani<sup>1</sup>; <sup>1</sup>Laboratoire de Spectrométrie de Masse BioOrganique, Université de Strasbourg, CNRS, IPHC UMR 7178, 67000, STRASBOURG, France; <sup>2</sup>IRPF, Centre d'Immunologie Pierre-Fabre (CIPF), 74160, Saint-Julien-en-Genevois, France



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- WP 482 **New High Resolution Mass Spectrometry Ion Mobility Applications in the Identification of Challenging Environmental Metabolites;** Yelena A. Adelfinskaya<sup>1</sup>; David G McCaskill<sup>1</sup>; Jesse L Balcer<sup>1</sup>; Nick N Wang<sup>1</sup>; Jeffery Gilbert<sup>1</sup>; Michael W. Madary<sup>1</sup>; Pete L. Johnson<sup>1</sup>; Suresh Annangudi Palani<sup>1</sup>; Scott A. Greenwalt<sup>1</sup>; <sup>1</sup>*Corteva Agriscience, Indianapolis, IN*
- WP 488 **Analysis of gold-molybdenum complexes by nano-electrospray ionization-ion mobility-mass spectrometry;** Hannah J Harbin<sup>1</sup>; Kyle L Wilhelm<sup>1</sup>; Dhiringam Humaidy<sup>2</sup>; Raul Villacob<sup>1</sup>; Alice E Bruce<sup>2</sup>; Mitchell R. M. Bruce<sup>2</sup>; Touradj Solouki<sup>1</sup>; <sup>1</sup>*Baylor University, Waco, TX*; <sup>2</sup>*The University of Maine, Orono, ME*
- WP 501 **Direct LC/MS analysis method of surfactants contained in antibody drugs using a polymer-based reversed phase column;** Leah Sullivan<sup>1</sup>; Junji Sasuga<sup>1</sup>; Hiroki Takenaka<sup>1</sup>; Eiji Kagawa<sup>1</sup>; Ron Benson<sup>1</sup>; <sup>1</sup>*Shodex, Showa Denko America, Inc., New York, NY*
- WP 510 **A new LC-MS Approach for Synthetic Peptide Characterization and Impurity Profiling;** Asish Chakraborty<sup>1</sup>; Nilini Nilini Ranbaduge<sup>1</sup>; Ying Qing Yu<sup>1</sup>; <sup>1</sup>*Waters Corporation, Milford, MA*
- WP 511 **Becoming street-smart in the CDMO space: utilization of multiple technologies to harmonize release and characterization assays for non-mAb proteins;** Irina Perdivara<sup>1</sup>; Margo Wilson<sup>1</sup>; Clara Smith<sup>1</sup>; <sup>1</sup>*Fujifilm Diosynth Biotechnologies, Morrisville, NC*
- WP 513 **A quantitative compliant Multi Attribute Methodology (MAM) LC/MS workflow;** Zoe Zhang<sup>1</sup>; Sean Mccarthy<sup>2</sup>; Elliott Jones<sup>1</sup>; Todd Stawicki<sup>2</sup>; <sup>1</sup>*Sciex, Redwood City, CA*; <sup>2</sup>*Sciex, Framingham, MA*
- WP 514 **A Sensitive Microflow LC/MS/MS Method for the Analysis of Corticosteroids in Human Plasma;** Ting Liu<sup>1</sup>; Wenhai Jin<sup>1</sup>; Daniel K Blake<sup>2</sup>; <sup>1</sup>*Sciex, Shanghai, China*; <sup>2</sup>*SCIEX, Warrington, United Kingdom*
- WP 519 **A comparative analysis of two sample preparation methods for the multi-omic analysis of proteins, lipids, and metabolites;** Melissa R Pergande<sup>1,2</sup>; Sheher Banu Mohsin<sup>2</sup>; Limian Zhao<sup>3</sup>; Stephanie M Cologna<sup>1</sup>; <sup>1</sup>*University of Illinois at Chicago, Chicago, IL*; <sup>2</sup>*Agilent Technologies, Wood Dale, IL*; <sup>3</sup>*Agilent Technologies, Inc., Wilmington, DE*
- WP 527 **Automating the analysis of estrogens in plasma using a multi-purpose auto-sampler coupled to liquid chromatography triple quadrupole mass spectrometry;** Mary Blackburn; *Thermo Fisher Scientific, San Jose, CA*
- WP 536 **Development and validation of LC-MS/MS method for determining Temozolomide in mouse brain following intra-cerebral microdialysis;** Raghavi Kakarla<sup>1</sup>; Kimberly Yacoub<sup>1</sup>; Baochuan Guo<sup>1</sup>; <sup>1</sup>*Cleveland State University, Cleveland, OH*
- WP 539 **Comparison of SPE Protocols for Phospholipid Removal in Basic Analyte Bioanalytical Quantitation;** Melvin Blaze Muttikal Thomas<sup>1</sup>; Thomas H Walter<sup>1</sup>; Kenneth Berthelette<sup>1</sup>; Bonnie A Alden<sup>1</sup>; Donna Osterman<sup>1</sup>; Kevin Wyndham<sup>1</sup>; <sup>1</sup>*Waters Corporation, Milford, MA*
- WP 543 **Mechanism of prostaglandin E2 accumulation in amniotic fluid during human labor;** Toshiaki Okuno<sup>1</sup>; Nanase Takahashi<sup>1</sup>; Takehiko Yokomizo<sup>1</sup>; <sup>1</sup>*Department of Biochemistry, Juntendo University School of Medicine, Tokyo, Japan*
- WP 545 **Investigating enzymatic lipase activity via contained-electrospray ionization (ESI) mass spectrometry as a function of secondary organic aerosol (SOA) evolution;** Mickey M. Rogers<sup>1</sup>; Benjamin J. Burris<sup>1</sup>; Abraham K. Badu-Tawiah<sup>1</sup>; <sup>1</sup>*The Ohio State University, Columbus, OH*
- WP 549 **Acute-phase Serum Lipidome Alterations in a Rodent Model of Closed Head Traumatic Brain Injury;** Scott Hogan<sup>1</sup>; Kyle Milligan<sup>2</sup>; Michelle LaPlaca<sup>2</sup>; Facundo M Fernandez<sup>1</sup>; <sup>1</sup>*Georgia Institute of Technology, School of Chemistry and Biochemistry, Atlanta, Georgia*; <sup>2</sup>*Georgia Institute of Technology, Department of Biomedical Engineering, Atlanta, Georgia*
- WP 556 **Lipid profiling of Chromochloris zofingiensis photoautotrophic and heterotrophic cultures;** Yuntao Hu<sup>1,2</sup>; Melissa S Roth<sup>2</sup>; Katherine Louie<sup>1,3</sup>; Benjamin Bowen<sup>1,3</sup>; Krishna Niyogi<sup>2</sup>; Trent Northen<sup>1,3</sup>;



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- <sup>1</sup>Lawrence Berkeley Laboratory, Berkeley, CA; <sup>2</sup>University of California, Berkeley, Berkeley, CA; <sup>3</sup>Joint Genome Institute, WALNUT CREEK, CA
- WP 558 **High speed untargeted lipidomics and metabolomics LC-MS/MS workflows with Parallel Accumulation Serial Fragmentation (PASEF);** Ulrike Schweiger-Hufnagel<sup>1</sup>; Aiko Barsch<sup>1</sup>; Sven W. Meyer<sup>1</sup>; <sup>1</sup>Bruker Daltonics, Bremen, Germany
- WP 559 **The regulation of the molecular structural diversity of mitochondrial cardiolipins in mouse tissues;** Gregor Oemer<sup>1</sup>; Jakob Koch<sup>2</sup>; Mohammed Tauqeer Alam<sup>3</sup>; Marie-Luise Edenhofer<sup>2</sup>; Sabrina Sailer<sup>4</sup>; Carolina Doerrier<sup>5</sup>; Ernst R Werner<sup>4</sup>; Katrin Watschinger<sup>4</sup>; Erich Gnaiger<sup>5</sup>; Johannes Zschocke<sup>2</sup>; Markus A Keller<sup>2</sup>; <sup>1</sup>Division of Human Genetics, Medical University of Innsbruck, Innsbruck, Austria; <sup>2</sup>Division of Human Genetics, Medical University of Innsbruck, Innsbruck, Austria; <sup>3</sup>Division of Biomedical Sciences, Warwick Medical School, University of Warwick, Warwick, United Kingdom; <sup>4</sup>Division of Biological Chemistry, Biocenter, Medical University of Innsbruck, Innsbruck, Austria; <sup>5</sup>Oroboros Instruments Corporation, Innsbruck, Austria
- WP 561 **Mass spectrometric study on the source of error in quantification of free fatty acids;** Hyejin Park<sup>1</sup>; Tae-Young Kim<sup>1</sup>; <sup>1</sup>School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology, Gwangju, South Korea
- WP 567 **Effects of acute ambient PM2.5 exposure on heart in C57BL/6J diet-induced obesity mouse model;** Yuanyuan Song<sup>1</sup>; Yanhao Zhang<sup>1</sup>; Zenghua Qi<sup>2</sup>; Ruijin Li<sup>3</sup>; Zongwei Cai<sup>1</sup>; <sup>1</sup>Hong Kong Baptist University, Hong Kong, China; <sup>2</sup>Guangdong University of Technology, Guangzhou, China; <sup>3</sup>Shanxi University, Taiyuan, China
- WP 572 **Isotope-labeled metabolic flux analysis of the gut microbiota-driven carnitine metabolism;** Hsin-bai Zou<sup>1</sup>; Fang-Wei Kuo<sup>2</sup>; Qiang Lyu<sup>3</sup>; Hsin-Yuan Chang<sup>3</sup>; Cheng-Chih Hsu<sup>3</sup>; Wei-Kai Wu<sup>4</sup>; <sup>1</sup>Department of Chemistry, National Taiwan University, Taipei, Taiwan; <sup>2</sup>Institute of food science and technology, Taipei, Taiwan; <sup>3</sup>Department of Chemistry, National Taiwan University, Taipei, Taiwan; <sup>4</sup>Department of Internal Medicine, National Taiwan University Hospital Bei-Hu Branch, Taipei, Taiwan, Taipei, Taiwan
- WP 573 **Multiplexed high throughput LC-MS/MS method for targeted metabolites and neurotransmitters from central nervous system;** Juho Heininen<sup>1</sup>; Tapio Kotiaho<sup>1</sup>; Anu Vaikkinen<sup>1</sup>; Risto Kostianen<sup>1</sup>; <sup>1</sup>University of Helsinki, Helsinki, Finland
- WP 580 **Direct Quantification of Polyamines in Arabidopsis thaliana seedlings by LC-MS/MS;** Masoud Zabet Moghaddam<sup>1</sup>; parvin mirzaei<sup>2</sup>; mohamed Fokar<sup>2</sup>; Yehia Mechref<sup>3</sup>; <sup>1</sup>Texas Tech University, Box 43132 Lubbock, TX; <sup>2</sup>Texas Tech University, Lubbock, TX; <sup>3</sup>Texas Tech University, Lubbock
- WP 582 **Reovirus-Induced Alterations in the Metabolome of M1 and M2 Macrophages;** Michael Giacomantonio<sup>1</sup>; Patrick J Murphy<sup>1</sup>; Barry Kennedy<sup>1</sup>; Shashi Gujar<sup>1,2</sup>; <sup>1</sup>Department of Pathology, Dalhousie University, Halifax, NS, Canada, Halifax, NS; <sup>2</sup>Department of Microbiology and Immunology, Dalhousie University, Halifax, NS, Canada, Halifax, NS, Canada, Halifax, NS
- WP 587 **Measurement of Metabolites in Feces of Japanese Rock Ptarmigans by LC-MS/MS;** Takanari Hattori<sup>1</sup>; Yukari Oka<sup>1</sup>; Shuichi Kawana<sup>1</sup>; Koretsugu Ogata<sup>1</sup>; Sayaka Tsuchida<sup>2,3</sup>; Atsushi Kobayashi<sup>4</sup>; Yoshiaki Nakamura<sup>5</sup>; Hiroshi Nakamura<sup>6</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>Kyoto Prefectural University, Kyoto, Japan; <sup>3</sup>Chubu University, Kasugai, Japan; <sup>4</sup>Toho University, Tokyo, Japan; <sup>5</sup>Hiroshima University, Hiroshima, Japan; <sup>6</sup>Nakamura Hiroshi International Institute for Ornithology, Nagano, Japan
- WP 588 **Rapid Throughput Quantitation of Carboxylic Acid Metabolites Using UHPLC/QqQ-MS to Monitor Diet and the Microbiome;** Diane Tu<sup>1</sup>; Carol Stroble<sup>1</sup>; Matthew J. Amicucci<sup>1</sup>; Gege Xu<sup>1</sup>; Jennifer T Smilowitz<sup>1</sup>; Carlito B Lebrilla<sup>1</sup>; <sup>1</sup>University of California, Davis, Davis, CA
- WP 590 **Simultaneous Detection of Tricarboxylic Acid Cycle Intermediates using LC-MS/MS with a Synergi® Fusion-RP HPLC Column;** Xianrong (Jenny) Wei<sup>1</sup>; Ryan Splitsstone<sup>1</sup>; Sean Orłowicz<sup>1</sup>; <sup>1</sup>Phenomenex, Torrance, CA



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- WP 598 **Untargeted metabolomics profiling of longitudinal urine samples collected from individual participant of integrated personalized omics profiling (iPOP) project;** Songjie Chen<sup>1</sup>; Liang Liang<sup>1</sup>; Yuqin Dai<sup>2</sup>; Michael Snyder<sup>1</sup>; <sup>1</sup>Stanford University, Stanford, CA; <sup>2</sup>Agilent, Santa Clara, CA
- WP 609 **Development and application of a novel metabolomics platform based on capillary electrophoresis coupled with a high-resolution mass spectrometry;** Kazunori Sasaki<sup>1</sup>; Hitoshi Sagawa<sup>1</sup>; Makoto Suzuki<sup>1</sup>; Kaori Abe<sup>1</sup>; Satoshi Ito<sup>2</sup>; Tsutomu Negama<sup>2</sup>; Moon-Il Kang<sup>1</sup>; Kenjiro Kami<sup>1</sup>; <sup>1</sup>Human Metabolome Technologies, Tsuruoka, Japan; <sup>2</sup>Sekisui Medical Company, Chuo-ku, Japan
- WP 610 **Comparison of data-dependent acquisition methods on an Orbitrap ID-X;** Kevin Y Cho<sup>1</sup>; Fuad J Naser<sup>1</sup>; Michaela Schwaiger-haber<sup>1</sup>; Miriam Sindelar<sup>1</sup>; Gary J Patti<sup>1</sup>; <sup>1</sup>Washington University in St. Louis, St. Louis, MO
- WP 615 **MDM2 Copy Number Aberrations Alter Ceramide Glycosylation in Liposarcoma Tumors, Impacting Drug Response;** Andrew Patt<sup>1</sup>; Bryce Demoret<sup>1</sup>; Andrew Patterson<sup>2</sup>; Philip Smith<sup>2</sup>; Ewy Mathe<sup>1</sup>; James Chen<sup>1</sup>; <sup>1</sup>The Ohio State University, Columbus, OH; <sup>2</sup>Pennsylvania State University, State College, PA
- WP 624 **Investigation of the formation and structure characteristics of miR-92a G-quadruplex by ESI-MS;** Min Xi<sup>1, 2</sup>; Jiang Zhou<sup>1</sup>; Yizhou Li<sup>2</sup>; <sup>1</sup>College of Chemistry and Molecular Engineering, Peking University, Beijing, China; <sup>2</sup>School of Pharmaceutical Sciences, Chongqing University, Shapingba, China
- WP 639 **Charge Deconvolution and Automatic Sequence Matching for Oligonucleotides;** Wilfred Tang<sup>1</sup>; Marshall Bern<sup>1</sup>; Rose D Lawler<sup>1</sup>; James Moore<sup>1</sup>; David Garby<sup>2</sup>; Nicholas Skizim<sup>2</sup>; <sup>1</sup>Protein Metrics Inc., Cupertino, CA; <sup>2</sup>GreenLight Biosciences, Inc., Medford, MA
- WP 644 **Identification of Glutamic Acid Isomers Produced During Deamidation Through RDD Diagnostic Fragments;** Jacob W Silzel<sup>1</sup>; Yana Lyon<sup>1</sup>; Dylan Riggs<sup>1</sup>; Ryan R. Julian<sup>1</sup>; <sup>1</sup>UC Riverside, Riverside, CA
- WP 653 **Expanding the glycoforms detected in complex glycopeptide datasets;** Katalin F. Medzihradzsky<sup>1</sup>; Peter R. Baker<sup>2</sup>; Adam Pap<sup>1</sup>; Zsuzsanna Darula<sup>1</sup>; Robert Chalkley<sup>2</sup>; <sup>1</sup>Biological Research Centre of the Hungarian Academy of Sciences, Szeged, Hungary; <sup>2</sup>UCSF, San Francisco, CA
- WP 654 **Highly Efficient and Precise Glycoproteomic Analysis with Intelligent Technology;** Weiqian Cao<sup>1</sup>; Wenfeng Zeng<sup>2</sup>; Mingqi Liu<sup>1</sup>; Chao Liu<sup>2</sup>; Biyun Jiang<sup>1</sup>; Pan Fang<sup>1</sup>; Huali Shen<sup>1</sup>; Simin He<sup>2</sup>; Pengyuan Yang<sup>1</sup>; <sup>1</sup>Fudan University, Shanghai, China; <sup>2</sup>Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China
- WP 674 **Pinpointing Isomerization Sites in Human Lens Crystallin using IMS-MS;** Hoi Ting Wu<sup>1</sup>; Ryan R. Julian<sup>1</sup>; <sup>1</sup>University of California, Riverside, Riverside, CA
- WP 676 **Blood brain barrier (BBB) penetration of pituitary adenylate cyclase-activating polypeptide (PACAP) glycosylated peptides by 'shotgun microdialysis' coupled with LC-MS3;** Chenxi Liu<sup>1</sup>; Mitchell J Bartlett<sup>2</sup>; Christopher Robert Apostol<sup>1</sup>; Lajos Szabo<sup>1</sup>; Robin Polt<sup>1</sup>; Torsten Falk<sup>2</sup>; Michael L Heien<sup>1</sup>; <sup>1</sup>Department of Chemistry and Biochemistry, The University of Arizona, Tucson, Arizona; <sup>2</sup>Department of Neurology, The University of Arizona, Tucson, Arizona
- WP 684 **Factors that influence the recovery of hydrophobic peptides during LC-MS sample handling;** Moon Chul Jung<sup>1</sup>; Kim Haynes<sup>1</sup>; Markus Wanninger<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA
- WP 686 **Sequential Windowed Acquisition of Reporter Masses for Quantitation-First Proteomics;** William D. Barshop<sup>1</sup>; Hee Jong Kim<sup>1</sup>; Shima Rayatpisheh<sup>1</sup>; James A. Wohlschlegel<sup>1</sup>; <sup>1</sup>University of California Los Angeles, Los Angeles, CA
- WP 688 **Developing fit-for-purpose LC-MS based quantitative assays to support drug discovery activities for cyclic peptides;** Rena N Zhang<sup>1</sup>; Michelle R Robinson<sup>2</sup>; Komal Kedia<sup>2</sup>; Daniel Spellman<sup>2</sup>; <sup>1</sup>Merck & Co., Inc, West Point, PA; <sup>2</sup>Merck & Co., Inc., West Point, PA
- WP 692 **Assay of Human Insulin by Liquid Chromatography High Resolution Mass Spectrometry;** Kui Zeng<sup>1</sup>; Jingyue Yang<sup>1</sup>; Connie Ruzicka<sup>1</sup>; <sup>1</sup>FDA, Saint Louis, MO





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- WP 703 **Development of a Very Sensitive LC-MS Assay to Quantitate Ultra Low Levels of GLP-1 Targeted Peptide Mimetics;** Jennifer Luong<sup>1</sup>; Jeremy Brassard<sup>1</sup>; Alyssa Kabat<sup>1</sup>; Eric Schnieder<sup>2</sup>; Allysen Meymaris<sup>1</sup>; Steven Wiltshire<sup>1</sup>; Jakal Amin<sup>1</sup>; <sup>1</sup>Charles River Laboratories, Worcester, MA; <sup>2</sup>ProLynx LLC, San Francisco, CA
- WP 707 **Thyroglobulin as a Model for Analysis of Protein Quality Control Dynamics;** Madison T. Wright<sup>1</sup>; Lars Plate<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN
- WP 708 **TRIM28 as a candidate mutant p53 interacting partner in cancer cells;** Mariel R Mendoza<sup>1</sup>; Katherine Alexander<sup>1</sup>; Enrique Lin Shiao<sup>1</sup>; Charly Ryan Good<sup>1</sup>; Benjamin A. Garcia<sup>1</sup>; Shelley L. Berger<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia
- WP 709 **Analysis of the lysosomal membrane interactome via cross-linking mass-spectrometry;** Jasjot Singh<sup>1</sup>; Sriganayatri Ponnaiyan<sup>1</sup>; Fatema Akter<sup>1</sup>; Dominic Winter<sup>1</sup>; <sup>1</sup>University of Bonn - Institute of Biochemistry and Molecular Biology, Bonn, Germany
- WP 717 **A cross-linking-aided IP/MS workflow reveals extensive intracellular trafficking in time-resolved, signal-dependent EGFR proteome;** Yue Chen<sup>1</sup>; Mei Leng<sup>1</sup>; Yankun Gao<sup>2</sup>; Jongmin Choi<sup>1</sup>; Dongdong Zhan<sup>2</sup>; Jun Qin<sup>1,2</sup>; Sung Yun Jung<sup>1</sup>; Yi Wang<sup>1,2</sup>; <sup>1</sup>Department of Biochemistry and Molecular Biology, Baylor College of Medicine, Houston, TX; <sup>2</sup>National Center for Protein Sciences (Beijing), State Key Laboratory of Proteomics, Institute of Lifeomics, Beijing, China
- WP 724 **Development of label free quantitative method for proteomics and its validation through interlab study;** Ki Na Yun<sup>1,2</sup>; Geul Bang<sup>1,3</sup>; Gun Wook Park<sup>1</sup>; Heeyoun Hwang<sup>1</sup>; Hongkyeong Jung<sup>1</sup>; Hye-Jung Kim<sup>4</sup>; Eugene Lee<sup>5</sup>; Yong-In Kim<sup>5</sup>; Jeong Hee Moon<sup>6</sup>; Sungho Yun<sup>7</sup>; Jong Shin Yoo<sup>1</sup>; Jin Young Kim<sup>1</sup>; <sup>1</sup>Biomedical Omics Group, Korea Basic Science Institute, Cheongju, South Korea; <sup>2</sup>Department of Chemistry, Sogang University, Mapo-gu, South Korea; <sup>3</sup>College of Pharmacy, Korea University, Jochiwon, South Korea; <sup>4</sup>New Drug Development Center, KBIO Osong Medical Innovation Foundation, Cheongju, South Korea; <sup>5</sup>Korea Research Institute of Standards and Science, Yuseong-gu, South Korea; <sup>6</sup>Disease Target Structure Research Center, KRIBB, Yuseong-gu, South Korea; <sup>7</sup>Drug and disease target research team, Korea Basic Science Institute, Cheongju, South Korea
- WP 735 **Optimizing injection time predictions to improve isobaric reagent reporter ion yield during multiplexed quantitative proteomic experiments;** Craig Braun<sup>1</sup>; Ryan Kunz<sup>1</sup>; Alison Erickson<sup>1</sup>; Steven P Gygi<sup>2</sup>; Brian Erickson<sup>1</sup>; <sup>1</sup>IQ Proteomics LLC, Cambridge, MA; <sup>2</sup>Harvard Medical School, Boston, MA
- WP 736 **Reporter Ion Cross-Channel Signals in TMT Multiplexing for the Carrier/Reference Strategy;** Paul Stemmer<sup>1</sup>; Nicholas J. Carruthers<sup>1</sup>; Joseph A Caruso<sup>1</sup>; David M. Lubman<sup>2</sup>; Zhijing Tan<sup>2</sup>; <sup>1</sup>Wayne State University, Detroit, MI; <sup>2</sup>University of Michigan, Ann Arbor, MI
- WP 741 **A Filter-Assisted Approach for Rapid Proteomic Sample Quality Estimation;** Jair T Montford<sup>1</sup>; Wenjing Peng<sup>1</sup>; Jingfu Zhao<sup>1</sup>; Aiying Yu<sup>1</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>Texas Tech University, Lubbock, TX
- WP 742 **Proteomic Analysis of Plasma – Sample Preparation and Multiplexing Workflows for Relative Quantitation;** Sergei Snovida<sup>1</sup>; Yen-Chun Lai<sup>2</sup>; Amarjeet Flora<sup>1</sup>; Ryan D. Bomgarden<sup>1</sup>; John C Rogers<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Rockford, IL; <sup>2</sup>Indiana University School of Medicine, Indianapolis, IN
- WP 751 **Overcoming challenges to develop a robust method for quantifying urinary mono-hydroxylated polycyclic aromatic hydrocarbons (OH-PAHs) by on-line SPE-LC-MS;** Yuesong Wang<sup>1</sup>; Erin N. Pittman<sup>1</sup>; Debra A. Trinidad<sup>1</sup>; Hei Sio Ao<sup>1</sup>; Antonia M. Calafat<sup>1</sup>; Julianne C. Botelho<sup>1</sup>; <sup>1</sup>CDC, Atlanta, GA
- WP 755 **Analysis of Propylene Glycol in Rat Plasma after Derivatization using Liquid Chromatography Coupled with Tandem Mass Spectrometric Detection (LC-MS/MS);** Changyu Quang<sup>1</sup>; William C. Nethero<sup>1</sup>; Donald B. Giroux<sup>1</sup>; Liam Moran<sup>1</sup>; Elizabeth A Groeber<sup>1</sup>; <sup>1</sup>Charles River, Ashland, OH
- WP 763 **Method Validation for the Determination of Novel Psychoactive Substances in Human Urine by Liquid Chromatography/High Resolution Mass Spectrometry;** Amber Awad<sup>1</sup>; Ana Celia Grenier<sup>1</sup>; Lawrence J Andrade<sup>1</sup>; <sup>1</sup>Dominion Diagnostics, North Kingstown, RI



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- WP 774 **Urine Pain Panel Drug Screen for 42 Analytes with Enzyme Hydrolysis and an Internal Hydrolysis Indicator in Each Patient Sample;** Stephen D Merrigan<sup>1</sup>; Gwendolyn A McMillin<sup>1,2</sup>; <sup>1</sup>ARUP Institute for Clinical and Experimental Pathology, Salt Lake City, UT; <sup>2</sup>University of Utah Health Sciences Center, Department of Pathology, Salt Lake City, UT
- WP 780 **Evaluating the tolerance mechanism of zebrafish embryo to spermidine carbon quantum dots by proteomics analysis;** YuJu Chen<sup>1</sup>; Pang-Hung Hsu<sup>2</sup>; Han-Jia Lin<sup>2</sup>; <sup>1</sup>National Yang-Ming University, Taipei, Taiwan; <sup>2</sup>National Taiwan Ocean University, Keelung, Taiwan
- WP 782 **Quantitation of Total Carbamazepine and Carbamazepine Epoxide in Serum/Plasma on HPLC-MS/MS;** Diane Ly<sup>1</sup>; Kamisha L. Johnson-Davis<sup>1,2</sup>; <sup>1</sup>ARUP Institute for Clinical and Experimental Pathology, Salt Lake City, UT; <sup>2</sup>University of Utah Health Sciences Center, Department of Pathology, Salt Lake City, UT
- WP 784 **Small Molecules Automated Extraction from Human Breast Milk Using the Extrahera and the EVOLUTE Express CX Prior to LC-MS/MS Analysis;** Mohamed Youssef<sup>1</sup>; Stephanie Marin<sup>1</sup>; Jillian Neifeld<sup>1</sup>; Jeremy Smith<sup>1</sup>; Mario Merida<sup>1</sup>; Elena Gairloch<sup>1</sup>; <sup>1</sup>Biotage, Charlotte, NC
- ThP 001 **Molecular Profiling of Cyanobacteria under Environmental Stimuli using Laser Ablation Electrospray Ionization Coupled with Ion Mobility Separation Mass Spectrometry;** Gessica Vasconcelos<sup>1</sup>; Sylwia A Stopka<sup>2</sup>; Boniek G Vaz<sup>1</sup>; Akos Vertes<sup>2</sup>; <sup>1</sup>Federal University of Goias, Goiania, Brazil; <sup>2</sup>George Washington University, Washington, DC
- ThP 004 **Detection of ricin and abrin toxin by laboratory-based and portable direct analysis in real-time mass spectrometry (DART-MS);** Jennifer W Sekowski<sup>1</sup>; Debora Van Der Riet-van Oeveren<sup>2</sup>; Ad De Jong<sup>2</sup>; Alex Fidder<sup>2</sup>; Paul S Demond<sup>1</sup>; Jacquelyn V Harris<sup>1</sup>; Daan Noort<sup>2</sup>; <sup>1</sup>U.S. Army RDECOM Chemical & Biological Center, Aberdeen Proving Ground, MD; <sup>2</sup>The Netherlands Organization, Rijswijk, Netherlands
- ThP 010 **Flavor release monitoring using direct analysis in real-time mass spectrometry on differentiate with respect to time;** Motoshi Sakakura<sup>1</sup>; Teruhisa Shiota<sup>1</sup>; Takehito Sagawa<sup>2</sup>; <sup>1</sup>AMR, Inc., Tokyo, Japan; <sup>2</sup>S&B foods Inc., Tokyo, Japan
- ThP 017 **Repeatability and practicality of PESI/MS/MS-based in vivo real-time monitoring system for hepatic/brain metabolites in living mice;** Kei Zaitzu<sup>1,2</sup>; Yumi Hayashi<sup>1,3</sup>; Tasuku Murata<sup>4</sup>; Kazumi Yokota<sup>4</sup>; Tomomi Ohara<sup>2</sup>; Hitoshi Tsuchihashi<sup>2</sup>; Akira Ishii<sup>2</sup>; Koretsugu Ogata<sup>4</sup>; Hiroshi Taninata<sup>4</sup>; <sup>1</sup>In Vivo Real-Time Omics Laboratory, Institute for Advanced Research, Nagoya University, Nagoya, Japan; <sup>2</sup>Department of Legal Medicine and Bioethics, Nagoya University Graduate School of Medicine, Nagoya, Japan; <sup>3</sup>Pathophysiological Laboratory Sciences, Department of Radiological and Medical Laboratory Sciences, Nagoya University Graduate School of Medicine, Nagoya, Japan; <sup>4</sup>Shimadzu Corporation, Kyoto, Japan
- ThP 021 **Extractable analysis of heart stem using HPLC Q-Tof mass spectrometry coupled with high resolution database and library;** Chang Jiang; , Chengdu, China
- ThP 028 **Areca alkaloids measured from buccal cells using DART-MS serve as accurate biomarkers for betel nut chewing;** Adrian Franke<sup>1</sup>; Laura Biggs<sup>2</sup>; Joanne Y. Yew<sup>3</sup>; Jennifer F Lai<sup>4</sup>; <sup>1</sup>Univ of Hawaii Cancer Ctr, Honolulu, HI; <sup>2</sup>University of Guam, Mangilao, Guam; <sup>3</sup>Pacific Biosciences Research Center, University of Hawaii, Honolulu, hawaii; <sup>4</sup>University of hawaii Cancer Center, Honolulu, Hawaii
- ThP 038 **Atmospheric pressure dark-current argon discharge ionization with comparable performance to direct analysis in real time mass spectrometry;** Teruhisa Shiota<sup>1</sup>; Kanako Sekimoto<sup>2</sup>; Motoshi Sakakura<sup>1</sup>; Mitsuo Takayama<sup>2</sup>; <sup>1</sup>AMR, Inc., Tokyo, Japan; <sup>2</sup>Yokohama City University, Yokohama, Japan
- ThP 045 **Solvent Assisted Surface Probe-Nanoelectrospray: A modular liquid-extraction based tool for combined top-down & bottom-up proteomic surface analysis;** Raul Villacob<sup>1</sup>; Luke T. Richardson<sup>1</sup>; Matthew Mulloy<sup>1</sup>; Touradj Solouki<sup>1</sup>; <sup>1</sup>Baylor University, Waco, TX
- ThP 046 **Laser desorption REIMS – the fundamentals and how they dictate applications and automation;** Emrys A Jones<sup>1</sup>; Daniel Simon<sup>2</sup>; Tamas Karancsi<sup>2</sup>; Danielle McDougall<sup>3</sup>; Csaba Hajdu<sup>2</sup>; Richard Schaffer<sup>2</sup>; Julia



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- ThP 051 **Balog<sup>2</sup>; Steven D Pringle<sup>4</sup>; Zoltan Takats<sup>5</sup>; <sup>1</sup>Waters, Wilmslow, United Kingdom; <sup>2</sup>Waters Research Center Kft., Budapest, Hungary; <sup>3</sup>Manchester Institute of Biotechnology, University of Manchester, United Kingdom; <sup>4</sup>Waters Corporation, Wilmslow, United Kingdom; <sup>5</sup>Imperial College, London, United Kingdom**  
**In Vivo Analysis of Plant Sap by Direct Sampling and Capillary Microsampling Electrospray Ionization Mass Spectrometry; Tina Tran<sup>1</sup>; Laith Z. Samarah<sup>1</sup>; Akos Vertes<sup>1</sup>; <sup>1</sup>George Washington University, Washington, DC**
- ThP 054 **Characterization of a Novel Plasma-Ionization Source for Real-Time Breath Analysis; Christopher Gongar<sup>1</sup>; Michael Wei<sup>1</sup>; Robin H.J Kemperman<sup>1</sup>; Richard A. Yost<sup>1</sup>; <sup>1</sup>University of Florida, Gainesville, FL**
- ThP 066 **Development of a Multiplatform Mass Spectrometry-Based Workflow for the In-Depth Structural Elucidation of Oligosaccharides and Polysaccharides; Juan J Castillo<sup>1</sup>; Ace G Galermo<sup>2</sup>; Matthew J Amicucci<sup>3</sup>; Eshani Nandita<sup>3</sup>; Carlito B Lebrilla<sup>3</sup>; <sup>1</sup>University of Davis, Davis, CA; <sup>2</sup>Univerisity of California, Davis, Davis, CA; <sup>3</sup>UC Davis, Davis, CA**
- ThP 072 **Deciphering key protein binding elements within short- and medium-length heparin oligomers using multidimensional chromatography followed by MS analysis; Cedric Bobst<sup>1</sup>; Igor A. Kaltashov<sup>1</sup>; <sup>1</sup>University of Massachusetts Amherst, Amherst, MA**
- ThP 077 **LC-MS/MS approach for the exploration of glycosylation as a gatekeeper for successful xenotransplantation; Myung Jin Oh<sup>1,2</sup>; Nari Seo<sup>1,2</sup>; Jaekyoung Ko<sup>1,2</sup>; Jinyoung Park<sup>1,2</sup>; Xi-jun Yin<sup>3</sup>; Jjindan Kang<sup>3</sup>; Hyun Joo An<sup>1,2</sup>; <sup>1</sup>Chungnam national university, Daejeon, South Korea; <sup>2</sup>Asia-Pacific Glycomics Reference Site, Daejeon, South Korea; <sup>3</sup>Yanbian University, Yanji, China**
- ThP 085 **A Method for the Rapid Determination of Polysaccharide Structures; Eshani Nandita<sup>1</sup>; Matthew J. Amicucci<sup>1</sup>; Ace G. Galermo<sup>1</sup>; Juan J. Castillo<sup>1</sup>; Carlito B. Lebrilla<sup>1</sup>; <sup>1</sup>UC Davis, Davis, CA**
- ThP 088 **Identification of Off-Target Protein-Small Molecule Interactions Using Cellular Thermal Shift Assay (CETSA) and Phase-Constrained Spectrum Deconvolution (?SDM) MS Data Acquisition; Clifford Phaneuf<sup>1</sup>; Antonius Koller<sup>2</sup>; Konstantin Aizikov<sup>3</sup>; Dmitry Grinfeld<sup>3</sup>; Arne Kreuzmann<sup>3</sup>; Daniel Mourad<sup>3</sup>; Oliver Lange<sup>3</sup>; Alexander A Makarov<sup>3</sup>; Lili Guo<sup>1</sup>; Harvey Lieberman<sup>1</sup>; Aharon Cohen<sup>1</sup>; Alexei Belenky<sup>1</sup>; Alexander R Ivanov<sup>2</sup>; <sup>1</sup>Sanofi, Waltham, MA; <sup>2</sup>Northeastern University, Boston, MA; <sup>3</sup>Thermo Fisher Scientific, Bremen, Germany**
- ThP 090 **Mapping Protein Interactions Using Data-Dependent Acquisition without Dynamic Exclusion; Shen Zhang<sup>1</sup>; Brett Larsen<sup>2</sup>; Cassandra Wong<sup>2</sup>; Anne-Claude Gingras<sup>2</sup>; <sup>1</sup>Lunenfeld-Tanenbaum Research Institute, Sinai Health System, Toronto; <sup>2</sup>Lunenfeld-Tanenbaum Research Institute, Sinai Health System, Toronto, ON**
- ThP 093 **Quantitative proteomic and phosphoproteomic elucidation of cancer aneuploidy; Alison M. Taylor<sup>1</sup>; Wenxue Li<sup>2</sup>; Sejal Jain<sup>1</sup>; Matthew Meyerson<sup>1</sup>; Yansheng Liu<sup>2,3</sup>; <sup>1</sup>Department of Medical Oncology, Dana-Farber Cancer Institute, Boston, MA 02115; <sup>2</sup>Yale Cancer Biology Institute, West Haven, CT 06516; <sup>3</sup>Department of Pharmacology, Yale University School of Medicine, New Haven, CT 06510**
- ThP 102 **Cysteine-DIA – the use of cysteine-containing peptides to increase the protein coverage in DIA; Muhammad Tahir<sup>1</sup>; Arkadiusz Nawrocki<sup>1</sup>; Martin Røssel Larsen<sup>1</sup>; <sup>1</sup>Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense, Denmark**
- ThP 103 **Effect of aerobic exercise on PBMC protein profile in insulin resistant (IR) and insulin sensitive (IS) participants; Kevin Paul Erazo Castillo<sup>1</sup>; Sara Ahadi<sup>1</sup>; Kevin Contrepois<sup>1</sup>; Fredrik Edfors<sup>1</sup>; Daniel Hornburg<sup>1</sup>; Si Wu<sup>1</sup>; Francois Haddad<sup>1</sup>; Michael Snyder<sup>1</sup>; <sup>1</sup>Stanford University, Stanford, CA**
- ThP 104 **Characterization of the Insolublome in Aging and Age-related Diseases using Mass Spectrometry with Data-Independent Acquisitions (DIA/SWATH); Xueshu Xie<sup>1</sup>; Manish Chamoli<sup>1</sup>; Dipa Bhaumik<sup>1</sup>; Kathleen Dumas<sup>1</sup>; Renuka Sivapatham<sup>1</sup>; Suzanne Angeli<sup>1</sup>; Anja Holtz<sup>1</sup>; Julie Andersen<sup>1</sup>; Birgit Schilling<sup>1</sup>; Gordon J. Lithgow<sup>1</sup>; <sup>1</sup>Buck Institute, Novato, CA**



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- ThP 107 **Employing Scanning SWATH to Support High Flow Proteomics Sample Acquisition;** Nic Bloomfield<sup>1</sup>; Gordana Ivošev<sup>1</sup>; Frasn Wasim<sup>1</sup>; Stephen Tate<sup>1</sup>; Christoph B Messner<sup>2</sup>; Vadim Demichev<sup>2</sup>; Spyros Vernardis<sup>2</sup>; <sup>1</sup>SCIEX, Concord, ON; <sup>2</sup>The Francis Crick Institute, London, United Kingdom
- ThP 114 **Early Detection Hepatocellular carcinoma via MRM-MS with a Serum Protein-based Multi-marker panel: A Large-Scale Multicenter study;** Injoon Yeo<sup>1</sup>; Hyunsoo Kim<sup>2,3,4</sup>; Ji Hyeon Lee<sup>5</sup>; Young-Suk Lim<sup>6,7</sup>; Youngsoo Kim<sup>2,5,8</sup>; <sup>1</sup>Departments of Biomedical Engineering, Seoul National University College of Medicine, Seoul, South Korea; <sup>2</sup>Departments of Biomedical Engineering, Seoul National University College of Medicine, Jongro-gu, South Korea; <sup>3</sup>Department of Biomedical Sciences, Seoul National University College of Medicine, Seoul, South Korea; <sup>4</sup>Institute of Medical and Biological Engineering, Medical Research Center, Seoul National University College of Medicine, Seoul, South Korea; <sup>5</sup>Department of Biomedical Sciences, Seoul National University College of Medicine, Jongro-gu, South Korea; <sup>6</sup>Department of Gastroenterology, University of Ulsan College of Medicine, Seoul, South Korea; <sup>7</sup>Liver center, Asan Medical Center, Seoul, South Korea; <sup>8</sup>Institute of Medical and Biological Engineering, Medical Research Center, Seoul National University College of Medicine, Jongro-gu, South Korea
- ThP 119 **Sex-Specific Protein Differences Linked to Alzheimer's Disease Risk Uncovered by a Coexpression-Regression Framework;** Erica S Modeste<sup>1</sup>; Eric B. Dammer<sup>1</sup>; Duc M Duong<sup>1</sup>; James J. Lah<sup>2</sup>; Allan I. Levey<sup>2</sup>; Aliza Wingo<sup>3</sup>; Thomas S Wingo<sup>2,4</sup>; Nicholas T. Seyfried<sup>1,2</sup>; <sup>1</sup>Department of Biochemistry, Emory University, Atlanta, GA; <sup>2</sup>Department of Neurology, Emory University, Atlanta, GA; <sup>3</sup>Department of Psychiatry and Behavioral Sciences, Emory University, Atlanta, Georgia; <sup>4</sup>Department of Human Genetics, Emory University, Atlanta, GA
- ThP 129 **Primary metabolomic and lipidomics profiling of blood plasma of pregnant patients with systemic lupus erythematosus;** Eun Mi Lee<sup>1</sup>; Seung Mi Lee<sup>2</sup>; Soo Jin Park<sup>1</sup>; Joong Shin Park<sup>2</sup>; Do Yup Lee<sup>1</sup>; <sup>1</sup>Kookmin University, Seoul, South Korea; <sup>2</sup>Seoul National University College of Medicine, Seoul, South Korea
- ThP 132 **Identification of potential reactive metabolite protein adducts using a LC-MS based non-targeted global metabolic profiling approach;** Xiaomeng Shen<sup>1</sup>; zhican wang<sup>1</sup>; Ruta Phadnis<sup>1</sup>; Dan A Rock<sup>1</sup>; Brooke M Rock<sup>1</sup>; <sup>1</sup>Amgen Inc., South San Francisco, CA
- ThP 146 **Application of Affinity Selection Mass Spectrometry in High-throughput Binder Confirmation;** Eric Shi<sup>1</sup>; Cynthia Chiu<sup>1</sup>; Steve Skinner<sup>1</sup>; Jeffrey Messer<sup>1</sup>; Eleanor Watts<sup>1</sup>; Joseph Franklin<sup>1</sup>; Jennifer Summerfield<sup>1</sup>; Kenneth Lind<sup>1</sup>; Cecil Rise<sup>1</sup>; Gang Yao<sup>1</sup>; <sup>1</sup>GSK, Cambridge, MA
- ThP 149 **Ultra-Fast Analysis of Intact Proteins Using SPE-TOF;** Caroline S. Chu<sup>1</sup>; Andy Gieschen<sup>2</sup>; Kevin McCann<sup>3</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>Agilent Technologies, Inc., Santa Clara, CA; <sup>3</sup>Agilent Technologies, Wood Dale, IL
- ThP 159 **Comparison of multiple steroid analysis between plasma and serum from postmenopausal women using validated LC-MS/MS methods;** Yuyong Ke<sup>1</sup>; Alain Dury<sup>1</sup>; Claude Labrie<sup>1</sup>; fernand labrie<sup>1</sup>; <sup>1</sup>EndoCeutics, Quebec, QC
- ThP 160 **Novel Diagnosis Technique for Identification of Asbestos Fibres in Mesothelioma Samples using LA-ICP-MS Imaging;** Oana M Voloaca<sup>1</sup>; Laura M Cole<sup>1</sup>; Malcolm R Clench<sup>1</sup>; Calum Greenhalgh<sup>2</sup>; Amy J Managh<sup>2</sup>; Sarah Haywood-Small<sup>1</sup>; <sup>1</sup>Sheffield Hallam University, Sheffield, United Kingdom; <sup>2</sup>Loughborough University, Loughborough, United Kingdom
- ThP 168 **A Novel Approach to Elemental Imaging: Laser Ablation – Inductively Coupled Plasma – Orbitrap Mass Spectrometry;** Mikhail Belov<sup>1</sup>; Lothar Rottmann<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific (Bremen), Bremen, Germany; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany
- ThP 177 **Adductomics: What are the potential sites of DNA attack by N-acetyl-p-benzoquinone imine (NAPQI) and benzoquinone?;** Siqi Li<sup>1</sup>; Michael Leeming<sup>1</sup>; Bun Chan<sup>2</sup>; Richard A. J. O'hair<sup>3</sup>; <sup>1</sup>University of



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*Melbourne, Melbourne, Australia; <sup>2</sup>Nagasaki University, Nagasaki, Japan; <sup>3</sup>University of Melbourne, Victoria, Australia*

- ThP 188 **Effects of long-term and trans-generational feeding transgenic corn to pure-line leghorn hens on the cecal microbiota and mucosal proteomics;** Ruqing Zhong<sup>1</sup>; Lilan Zhang<sup>1</sup>; Liang Chen<sup>1</sup>; Qingshi Meng<sup>1</sup>; Sheng Zhang<sup>2</sup>; Hongfu Zhang<sup>1</sup>; <sup>1</sup>State Key Laboratory of Animal Nutrition, Institute of Animal Science, Chinese Academy of Agricultural Sciences, Beijing, China; <sup>2</sup>Proteomics and Metabolomics Facility, Institute of Biotechnology, Cornell University, Ithaca, NY
- ThP 189 **Analysis of Volatile Compounds in Pumpkin with ‘Taro-like’ Aroma using Solid phase Micro-extraction and Gas Chromatography-Mass Spectrometry combined with chemometrics;** Junxing Li<sup>1,2</sup>; Yujuan Zhong<sup>1,2</sup>; Wenwen Wang<sup>3</sup>; Haibin Wu<sup>1,2</sup>; Jianning Luo<sup>1</sup>; Hao Gong<sup>1</sup>; Hexun Huang<sup>1</sup>; <sup>1</sup>Vegetable Research Institute, Guangdong Academy of Agricultural Sciences, Guangzhou, China; <sup>2</sup>Guangdong Key Laboratory for New Technology Research of Vegetables, Guangzhou, China; <sup>3</sup>Agilent Technologies Co. Ltd, Beijing, China
- ThP 192 **GC-MS Combined with Chemometrics Reveals the Difference in Volatile Metabolic Profile Between High Yield and Normal Yield Royal Jelly;** Dandan Qi<sup>1</sup>; Chengying Ma<sup>2</sup>; Wenwen Wang<sup>3</sup>; Jianke Li<sup>1</sup>; <sup>1</sup>Institute of Apicultural Research / Key Laboratory of Pollinating Insect Biology, Ministry of Agriculture, Chinese Academy of Agricultural Sciences, Beijing, China; <sup>2</sup>Tea Research Institute, Guangdong Academy of Agricultural Sciences, Guangzhou, China; <sup>3</sup>Agilent Technologies Co. Ltd, Beijing, China
- ThP 194 **High-Resolution mass spectrometry informs the selection of food processing parameters for the large-scale enzymatic release of N-glycans from milk glycoproteins;** Apichaya Bunyatratchata<sup>1</sup>; Yu-Ping Huang<sup>1</sup>; Gulustan Ozturk<sup>1</sup>; Juliana Maria Leite Nobrega De Moura Bell<sup>1</sup>; Daniela Barile<sup>1,2</sup>; <sup>1</sup>Department of Food Science and Technology, University of California, Davis, California; <sup>2</sup>Foods for Health Institute, University of California, Davis, California
- ThP 200 **Droplet-based Desorption of Trace Volatiles following Parallel Headspace Extraction onto Sorbent Sheets;** Madeleine Y Bee<sup>1</sup>; Jessica P Rafson<sup>1</sup>; Gavin L. Sacks<sup>1</sup>; <sup>1</sup>Cornell University, Ithaca, NY
- ThP 206 **Enzymatic Tagging of Glycoproteins on the Cell Surface for Their Global and Site-Specific Analysis with Mass Spectrometry;** Fangxu Sun<sup>1</sup>; Suttipong Suttapitugsakul<sup>1</sup>; Ronghu Wu<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA
- ThP 207 **An Effective Chemical Method to Catch Low-Abundance Glycoproteins for MS Analysis;** Ronghu Wu<sup>1</sup>; Haopeng Xiao<sup>1</sup>; Suttipong Suttapitugsakul<sup>1</sup>; Fangxu Sun<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA
- ThP 208 **Improved Profiling of Sialylated N-Linked Glycans by Ion Chromatography-Orbitrap Mass Spectrometry;** Sachin Patil<sup>1</sup>; Jeffrey Rohrer<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Sunnyvale, CA
- ThP 209 **Rapid Characterization of Domain-Specific [Fc vs. Fab] Glycosylation in Monoclonal Antibodies (mAbs);** Charles Nwosu<sup>1</sup>; Mei Zhu<sup>2</sup>; Lei Wang<sup>1</sup>; Anne Kowal<sup>1</sup>; <sup>1</sup>Takeda Pharmaceuticals International Co, Cambridge, MA; <sup>2</sup>Takeda Pharmaceuticals, International Co., Cambridge, MA
- ThP 210 **Glycoproteomic Analysis of Cells Containing Unnatural Monosaccharides;** Yixuan (Axe) Xie<sup>1</sup>; Ying Sheng<sup>1</sup>; Qiongyu Li<sup>1</sup>; Maurice Wong<sup>1</sup>; Qingwen (Dave) Zhou<sup>1</sup>; Carlito B. Lebrilla<sup>1</sup>; <sup>1</sup>University of California, Davis, Davis, CA
- ThP 211 **Simultaneously Identifying and Distinguishing Glycoproteins with O-GlcNAc and the Tn Antigen in Human Cancer Cells;** Senhan Xu<sup>1</sup>; Jiangnan Zheng<sup>1</sup>; Haopeng Xiao<sup>2</sup>; Ronghu Wu<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA; <sup>2</sup>Harvard Medical School, Boston, MA
- ThP 219 **Mass spectrometric elucidation of global glycosylation profile on a fungal vaccine adjuvant BL-ENG2;** Junfeng Huang<sup>1</sup>; Lucas dos Santos Dias<sup>2</sup>; Marcel Wüthrich<sup>2</sup>; Lingjun Li<sup>1,3</sup>; <sup>1</sup>School of Pharmacy, University of Wisconsin-Madison, Madison, WI 53705; <sup>2</sup>Department of Pediatrics, School of Medicine and Public Health, University of Wisconsin-Madison, MADISON, WI; <sup>3</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706



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- ThP 225 **Bifunctional cleavable probe for in-situ multiplexed glycan detection and imaging using mass spectrometry;** Wen Ma<sup>1</sup>; Shuting Xu<sup>1</sup>; Yu Bai<sup>1</sup>; Huwei Liu<sup>1</sup>; <sup>1</sup>*Peking University, Beijing, China*
- ThP 235 **Characterizing Malignancy Potential of Pancreatic Intraductal Papillary Mucinous Neoplasm (IPMN) Cyst Tissue and Fluid using Desorption Electrospray Ionization Mass Spectrometry;** Alena Bensussan<sup>1</sup>; John Lin<sup>1</sup>; Sadhna Dhingra<sup>2</sup>; Hop S Tran Cao<sup>3</sup>; Livia S. Eberlin<sup>1</sup>; <sup>1</sup>*The University of Texas at Austin, Austin, TX*; <sup>2</sup>*Baylor College of Medicine, Houston, TX*; <sup>3</sup>*MD Anderson Cancer Center, Houston, TX*
- ThP 239 **Comprehensive quantitative lipidomic analysis of mouse hearts using AP-SMALDI mass spectrometry imaging and LC-MS/MS;** Vannuruswamy Garikapati<sup>1, 2</sup>; Claudia Colasante<sup>2</sup>; Eveline Baumgart-Vogt<sup>2</sup>; Bernhard Spengler<sup>1</sup>; <sup>1</sup>*Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, Giessen, Germany*; <sup>2</sup>*Institute for Anatomy and Cell Biology II, Division of Medical Cell Biology, Justus Liebig University Giessen, Giessen, Germany*
- ThP 256 **A MULTIMODAL APPROACH USING DESI-MSI AND LASER CAPTURE MICRODISSECTION FOR SINGLE TISSUE SECTION ANALYSIS;** Emine Kazanc<sup>1</sup>; Evdoxia Karali<sup>2</sup>; Vincen Wu<sup>1</sup>; James Mckenzie<sup>1</sup>; Olof Isberg<sup>1</sup>; Andreas Dannhorn<sup>1</sup>; Paolo Inglese<sup>1</sup>; Sadaf Ghaem-Maghamsi<sup>3</sup>; George Poulogiannis<sup>2</sup>; Zoltan Takats<sup>1</sup>; <sup>1</sup>*Imperial College London, Department of Surgery and Cancer, United Kingdom*; <sup>2</sup>*Institute of Cancer Research, Division of Cancer Biology, United Kingdom*; <sup>3</sup>*Imperial College London, Hammersmith Hospital, London, United Kingdom*
- ThP 262 **In-situ nanoscale chemical characterization of polymer coating melting and crystallization via multimodal chemical imaging;** Anton levlev<sup>1, 2</sup>; Matthias Lorenz<sup>1, 2</sup>; Olga S Ovchinnikova<sup>3</sup>; <sup>1</sup>*Oak Ridge National Laboratory, Oak Ridge, TN*; <sup>2</sup>*University of Tennessee, Knoxville, Knoxville, TN*; <sup>3</sup>*Oak Ridge National Laboratory, Oak Ridge, Tennessee*
- ThP 263 **Tandem MS Imaging of (Sub-)Monolayer Coatings at High Spatial Resolving Power for Process Assessment in Device Fabrication;** Gregory L Fisher; *Physical Electronics, Chanhassen, MN*
- ThP 269 **Direct Scoring from DIA Data using High Connected Data Models;** Fras Wasim<sup>1</sup>; Cristiano Viega<sup>1</sup>; Stephen A Tate<sup>1</sup>; <sup>1</sup>*SCIEX, Concord, ON*
- ThP 270 **Enhanced scoring of DIA data extraction using Machine Learning;** Gillian Brooks<sup>1</sup>; Fras Wasim<sup>1</sup>; Stephen A Tate<sup>1</sup>; <sup>1</sup>*SCIEX, Concord, ON*
- ThP 278 **Evaluation of Ion Mobility-Assisted Data Independent Acquisition (UDMSE) for Metaproteomics Sample Analysis;** Lisa M Wolfe<sup>1</sup>; Kitty J. Brown<sup>1</sup>; Brad J Williams<sup>2</sup>; Giorgis Isaac<sup>3</sup>; Jessica E. Prenni<sup>1, 4</sup>; Corey D. Broeckling<sup>1</sup>; <sup>1</sup>*Proteomics & Metabolomics Facility, Colorado State University, Fort Collins, CO*; <sup>2</sup>*Waters Corporation, Beverly, MA*; <sup>3</sup>*Waters Corporation, Milford, MA*; <sup>4</sup>*Department of Horticulture & Landscape Architecture, Colorado State University, Fort Collins, CO*
- ThP 293 **Gas-Phase Unfolding Reveals Subtle Stability Shifts in Higher-Order Substrate-Cytochrome P450 Complexes;** Chunyi Zhao<sup>1</sup>; Kinshuk Srivastava<sup>2</sup>; David Sherman<sup>1, 2</sup>; Brandon T. Ruotolo<sup>1</sup>; <sup>1</sup>*Department of Chemistry, University of Michigan, Ann Arbor, MI*; <sup>2</sup>*Life Sciences Institute, University of Michigan, Ann Arbor, MI*
- ThP 307 **Conformational Diversity of Vasotocin Nonapeptide Diastereomers Revealed by Uniform Field and Cyclic Traveling Wave Ion Mobility-Mass Spectrometry Measurements;** Shawn T. Phillips<sup>1</sup>; Emanuel Zlibut<sup>1</sup>; Jody C. May<sup>1</sup>; John A. McLean<sup>1</sup>; Martin E. Palmer<sup>2</sup>; Dale A. Cooper-Shepherd<sup>2</sup>; James I. Langridge<sup>2</sup>; <sup>1</sup>*Vanderbilt University, Nashville, TN*; <sup>2</sup>*Waters Corporation, Wilmslow, United Kingdom*
- ThP 308 **Molecular classification and identification using tandem ion mobility spectrometry with neural networks analysis of mobility selected ions and full spectra;** Hossein Shokri<sup>1</sup>; Natividad Jurado-Campos<sup>2</sup>; Ben Gardner<sup>3</sup>; Niu Hsein-Chi W<sup>4</sup>; Erkinjon Nazarov<sup>1</sup>; Gary A. Eiceman<sup>1</sup>; <sup>1</sup>*New Mexico State University, Las Cruces, NM 88003*; <sup>2</sup>*University of Córdoba, Rabanales, Spain*; <sup>3</sup>*Collins Aerospace, 960 Overland Court, San Dimas, California 91773*; <sup>4</sup>*960 Overland Court, San Dimas, California 91773*



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- ThP 320 **INTRODUCING STRUCTURAL DETAIL IN ION MOBILITY SPECTRA OF ALCOHOLS AT AMBIENT PRESSURE USING A TANDEM DRIFT TUBE WITH REACTIVE STAGE;** Hossein Shokri<sup>1</sup>; Maika Vuki<sup>2</sup>; Ben Gardner<sup>3</sup>; Niu Hsein-Chi W<sup>4</sup>; Umesh Chiluwal<sup>1</sup>; Bhupendra Gurung<sup>1</sup>; David Emery<sup>1</sup>; Gary A. Eiceman<sup>1</sup>; Gyoungil Lee<sup>5</sup>; <sup>1</sup>New Mexico State University, Las Cruces, NM, 88003; <sup>2</sup>University of Guam, Mangilao, Guam, 96923; <sup>3</sup>Collins Aerospace, 960 Overland Court, San Dimas, California 91773; <sup>4</sup>960 Overland Court, San Dimas, California 91773; <sup>5</sup>New Mexico State University, Las Cruces, NM 88003
- ThP 322 **13C-Metabolic flux analysis of inhibitor-induced metabolic redirection in the central metabolism of breast cancer cells;** Fumio Matsuda<sup>1</sup>; Chie Araki<sup>1</sup>; Kousuke Maeda<sup>1</sup>; Nobuyuki Okahashi<sup>1</sup>; Hiroshi Shimizu<sup>1</sup>; <sup>1</sup>Osaka University, Suita, Japan
- ThP 333 **An alternative narrow-bore column to facilitate high-throughput “UHPLC” type and microflow LC-MS strategies for residue analysis;** Arianne Soliven<sup>1</sup>; Lucia Pareja<sup>2</sup>; Horacio Heinzen<sup>1</sup>; Andrés Pérez Parada<sup>1,3</sup>; <sup>1</sup>Grupo de Analisis de Compuestos Traza, Facultad de Química, Universidad de la Republica,, Montevideo, Uruguay; <sup>2</sup>Departamento de Química del Litoral, CENUR LO, Universidad de la República, Paysandú, Uruguay; <sup>3</sup>Departamento de Desarrollo Tecnológico, CURE, Universidad de la República, Rocha, Uruguay
- ThP 337 **Establish an analytical model for chemical preservatives using QTOF and MPP software;** Shaozhen Wang; Agilent Technologies, Shanghai, China
- ThP 338 **Hydrogen-Deuterium Exchange Liquid Chromatography / High Resolution Mass Spectrometry for Structure Elucidation of Unknown Organic Molecules;** Chengli Zu<sup>1</sup>; Renzo Samame<sup>1</sup>; Daniel Knueppel<sup>1</sup>; Jeffery Gilbert<sup>1</sup>; <sup>1</sup>Corteva Agriscience, Indianapolis, IN
- ThP 340 **Automatic detection of impurities and byproducts in complicated reactions using LC-HRMS;** Elisabeth Ortega-Carrasco<sup>1</sup>; Jenny Desantis<sup>2</sup>; Fabien Fontaine<sup>1</sup>; Blanca Serra<sup>1</sup>; Paolo Benedetti<sup>3</sup>; Ismael Zamora<sup>1,3</sup>; <sup>1</sup>Lead Molecular Design, S.L., Sant Cugat Del Valles, Spain; <sup>2</sup>University of Perugia, Perugia, Italy; <sup>3</sup>Molecular Discovery, London, United Kingdom
- ThP 341 **An integrated approach for the estimation of hazardous transformation products from metoprolol and metoprolol acid in UV/H<sub>2</sub>O<sub>2</sub> treated wastewaters;** Adrian Jaen-Gil<sup>1</sup>; Gianluigi Buttiglieri<sup>1</sup>; Aleix Benito<sup>2</sup>; Rafael Gonzalez-Olmos<sup>2</sup>; Sara Rodriguez-Mozaz<sup>1</sup>; Damia Barcelo<sup>1</sup>; <sup>1</sup>ICRA, Girona, Spain; <sup>2</sup>IQS School of Engineering, Universitat Ramon Llull, Barcelona, Spain
- ThP 352 **Application of 2D LC with MS Detection with Superficially Porous Columns to the Analysis of Cold Medicine;** William Long<sup>1</sup>; Anne E Mack<sup>2</sup>; Carl Griffin<sup>2</sup>; <sup>1</sup>Agilent Technologies, Wilmington, DE; <sup>2</sup>Agilent Technologies, Inc., Wilmington, DE
- ThP 353 **Assessing contamination in publicly available proteomic datasets;** Matthew Rardin<sup>1</sup>; Daryl Bulloch<sup>1</sup>; Bradford W. Gibson<sup>1</sup>; <sup>1</sup>Amgen, South San Francisco, CA
- ThP 358 **Comparison of Six Proteomics Sample Preparation Methods, Digestion Reagents and Proof of Principle Automation;** Aleksandr Gaun<sup>1</sup>; Sudha Gollapudi<sup>1</sup>; Rob Keyser<sup>1</sup>; Fiona McAllister<sup>1</sup>; <sup>1</sup>Calico Labs, South San Francisco, CA
- ThP 360 **Improving host cell protein profiling in biopharmaceuticals by advanced LC-MS/MS methods;** Regina Kufer<sup>1</sup>; Martina Suessmair<sup>1</sup>; Ingo Lindner<sup>1</sup>; Don Walker<sup>2</sup>; Christopher Yu<sup>2</sup>; Stefanie Wohlrab<sup>1</sup>; Markus Haindl<sup>1</sup>; Harald Wegele<sup>1</sup>; <sup>1</sup>Roche Diagnostics GmbH, Penzberg, Germany; <sup>2</sup>Genentech, South San Francisco, CA
- ThP 361 **A method to optimize proteome analyses of low cell numbers of pathogens retrieved from infection assays;** Manuela Gesell Salazar<sup>1</sup>; Sascha Blankenburg<sup>1</sup>; Christian Hentschker<sup>1</sup>; Denise Dittmar<sup>1</sup>; Petra Hildebrandt<sup>1</sup>; Stephan Michalik<sup>1</sup>; Anna Nagel<sup>1</sup>; Kristin Surmann<sup>1</sup>; Uwe Völker<sup>1</sup>; <sup>1</sup>University Medicine Greifswald, Greifswald, Germany
- ThP 364 **Development of Tissue Sample Preparation Method for Large-scale Quantitative Mass Spectrometry Analysis;** Yoseop Kim<sup>1</sup>; Hyunsoo Kim<sup>1,2,3</sup>; Minsoo Son<sup>1</sup>; Youngsoo Kim<sup>2,3,4</sup>; <sup>1</sup>Department of Biomedical



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- ThP 367 **High-temperature trypsin characterization and comparison;** Laura K. Muehlbauer<sup>1</sup>; Alexander S. Hebert<sup>2</sup>; Joshua J. Coon<sup>1,2,3,4</sup>; <sup>1</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, WI; <sup>2</sup>Genome Center of Wisconsin, Madison, WI; <sup>3</sup>Morgridge Institute for Research, Madison, WI; <sup>4</sup>Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI
- ThP 368 **Development of a SPE LC-MS/MS Method for the Bioanalytical Quantification of Pramlintide from Serum;** Caitlin M Dunning<sup>1</sup>; Mary E Lame<sup>1</sup>; Paula M Orens<sup>1</sup>; Kim Haynes<sup>1</sup>; Mark D Wrona<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA
- ThP 388 **Widely targeted lipidomics profiling (WTLP) with unit Dalton resolution using the Sciex 6500+ QTRAP;** Yunping Qiu<sup>1</sup>; Mackenzie J J Pearson<sup>2</sup>; Min Cai<sup>1</sup>; Cyrus Papan<sup>3</sup>; Irwin J Kurland<sup>4</sup>; <sup>1</sup>Albert Einstein College of Medicine, Bronx, NY; <sup>2</sup>Sciex, Framingham, MA; <sup>3</sup>SCIEX, Darmstadt, Germany; <sup>4</sup>Albert Einstein CollegeMed, Bronx, NY
- ThP 395 **Higher confidence annotations of target lipids enabled by Trapped Ion Mobility MS in combination with machine learning based CCS prediction;** Matthias Szesny<sup>1</sup>; Sebastian Wehner<sup>1</sup>; Heiko Neuweger<sup>1</sup>; Ulrike Schweiger-Hufnagel<sup>1</sup>; Sven W. Meyer<sup>1</sup>; Aiko Barsch<sup>1</sup>; Nikolas Kessler<sup>1</sup>; Lucy Woods<sup>1</sup>; <sup>1</sup>Bruker Daltonics, Bremen, Germany
- ThP 397 **A novel data strategy towards an integrated LC/MS- 1H NMR workflow for identifying unknown lipids;** Jiajun Lei<sup>1</sup>; Rohit Mahar<sup>1</sup>; Ram Khattri<sup>1</sup>; Matthew E. Merritt<sup>1</sup>; Timothy J. Garrett<sup>1</sup>; Richard A Yost<sup>1</sup>; <sup>1</sup>University of Florida, Gainesville, FL
- ThP 399 **Dual Derivatization Strategy for the LCMS Analysis of Plasmenyl Glycerophospholipids;** Samuel W Shields<sup>1</sup>; Carlos R Canez<sup>1</sup>; Peter J Pallister<sup>1</sup>; Jeffrey M Manthorpe<sup>1</sup>; Jeffrey C Smith<sup>1</sup>; <sup>1</sup>Carleton University, Ottawa, ON
- ThP 416 **High-Throughput MALDI-TOF Stem Cell Quality Assurance;** Stephen Zambrzycki<sup>1</sup>; Gilad Doron<sup>2</sup>; Johnna S Temenoff<sup>2</sup>; Facundo M Fernandez<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, School of Chemistry and Biochemistry, Atlanta, Georgia; <sup>2</sup>Georgia Institute of Technology, Department of Biomedical Engineering, Atlanta, Georgia
- ThP 432 **Integrated workflow with quality control for large cohort and clinical metabolomics research using robust hardware and signal correction;** Sebastian Goetz<sup>1</sup>; Ulrike Schweiger-Hufnagel<sup>1</sup>; Matthias Szesny<sup>1</sup>; Aiko Barsch<sup>1</sup>; Sven W. Meyer<sup>1</sup>; Matthew R. Lewis<sup>2</sup>; Nikolas Kessler<sup>1</sup>; <sup>1</sup>Bruker Daltonics, Bremen, Germany; <sup>2</sup>Imperial College London, London, United Kingdom
- ThP 433 **Dynamic Assessment of the Human Saliva Structural Lipidome using MS/MSALL Shotgun Lipidomics for Population Health Applications;** Valerie Bussberg<sup>1</sup>; Hannah Rockwell<sup>1</sup>; Gramoz Kondakci<sup>1</sup>; Emily Y. Chen<sup>1</sup>; Fei Gao<sup>1</sup>; Niven R. Narain<sup>1</sup>; Michael A. Kiebish<sup>1</sup>; <sup>1</sup>BERG, LLC, Framingham, MA
- ThP 434 **Development of a Functional Neurometabolomics Platform to Enable MOA and Functional Studies in Drug Development and Precision Medicine;** Bennett Greenwood<sup>1</sup>; Collin Hill<sup>1</sup>; Vladimir Tolstikov<sup>1</sup>; Reinhard Roessler<sup>1</sup>; Christine Denny<sup>2</sup>; Josephine McGowan<sup>2</sup>; Vivek Vishnudas<sup>1</sup>; Rangaprasad Sarangarajan<sup>1</sup>; Niven R. Narain<sup>1</sup>; Michael A. Kiebish<sup>1</sup>; <sup>1</sup>BERG, LLC, Framingham, MA; <sup>2</sup>Columbia University, New York, NY
- ThP 455 **Metabolomic profiling shows that glutathione depletion is rescued along with growth rate in yeast methionine auxotrophs;** Matthew A. Kukurugya<sup>1</sup>; Bernd J. Wranik<sup>1</sup>; Tina Mahatdejkul-Meadows<sup>1</sup>; R. Scott Mclsaac<sup>1</sup>; Bryson D. Bennett<sup>1</sup>; <sup>1</sup>Calico Life Sciences, South San Francisco, CA





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- ThP 459 **Modelling Cancer Lipogenesis using LA-REIMS Metabolic Flux analysis in breast cancer cell lines;** Seyma Turkseven<sup>1</sup>; Nikolaos Koundouros<sup>2</sup>; Simon Cameron<sup>3</sup>; Alvaro Perdones-Montero<sup>3</sup>; Renata Soares<sup>3</sup>; Luisa Doria<sup>3</sup>; George Poulogiannis<sup>2</sup>; Zoltan Takats<sup>3</sup>; <sup>1</sup>Imperial College London, London, United Kingdom; <sup>2</sup>Institute of Cancer Research, London, United Kingdom; <sup>3</sup>Imperial College, London, United Kingdom
- ThP 460 **Ion-Pair Selection Method for Pseudotargeted Metabolomics Based on SWATH MS Acquisition and Its Application in Type 2 Diabetes study;** Xinjie Zhao<sup>1,2</sup>; Lichao wang<sup>1,2</sup>; Benzhe Su<sup>3</sup>; Zhongda Zeng<sup>1</sup>; Chao Li<sup>3</sup>; Wangjie Lv<sup>1,2</sup>; Qihui Xuan<sup>1,2</sup>; Lina Zhou<sup>1,2</sup>; Xin Lu<sup>1,2</sup>; Xiaohui Lin<sup>1,2</sup>; Guowang Xu<sup>1,2</sup>; <sup>1</sup>CAS Key Laboratory of Separation Science for Analytical Chemistry, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China; <sup>2</sup>University of Chinese Academy of Sciences, Beijing, China; <sup>3</sup>School of Computer Science & Technology, Dalian University of Technology, Dalian, China
- ThP 467 **Quatitaion of glycine using LC-MS to investigate its role in sex-specific association with coronary heart diseases in vivo studies;** Ah Young Yoon<sup>1</sup>; Nicholas C. Woodward<sup>2</sup>; Janet Gukasyan<sup>2</sup>; Sujatha Chilakala<sup>1</sup>; Hooman Allayee<sup>2</sup>; Jonathan E Katz<sup>1</sup>; <sup>1</sup>Lawrence J. Ellison Institute for Transformative Medicine of USC, Los Angeles, California; <sup>2</sup>University of Southern California, Los Angeles, California
- ThP 468 **Integrating LC/MS-Based metabolomics and solid-state NMR for total accounting of carbon;** Miriam Sindelar<sup>1,2</sup>; Xiangfeng Niu<sup>1,2</sup>; Jacob Schaefer<sup>1</sup>; Brian N Finck<sup>2</sup>; Gary J Patti<sup>1,2</sup>; <sup>1</sup>Washington University in St. Louis, St. Louis; <sup>2</sup>Washington University School of Medicine in St. Louis, St. Louis, MO
- ThP 469 **Metabolic phylogeny: evidence for speciation through metabolic selection in the evolution of Borrelia, the causative agent of Lyme disease;** Ryan A Groves<sup>1</sup>; Thomas Rydzak<sup>1</sup>; Mildred Castellanos<sup>2</sup>; Peter Kraiczyn<sup>3</sup>; George Chaconas<sup>2</sup>; Ian A Lewis<sup>1</sup>; <sup>1</sup>Lewis Research Group, Department of Biological Sciences, University of Calgary, Calgary, AB; <sup>2</sup>Department of Biochemistry and Molecular Biology, University of Calgary, Calgary, AB; <sup>3</sup>Institute of Medical Microbiology and Infection Control, University Hospital of Frankfurt, Frankfurt Am Main, Germany
- ThP 472 **Cancer Cell Metabolism in KRAS Mice Revealed by Direct Sample Analysis with MALDI-TOF and High Resolution Mass Spectrometry;** Bo Wei<sup>1</sup>; Lin Tan<sup>1</sup>; Robyn Rhea<sup>1</sup>; Peiyong Yang<sup>1</sup>; <sup>1</sup>M D Anderson Cancer Center, Houston, TX
- ThP 477 **Rock varnish as a source of biosignatures for Mars extant life;** Hiro Teshima<sup>1</sup>; Chris M Yeager<sup>1</sup>; Nina L Lanza<sup>1</sup>; Ricardo Marti-Arbona<sup>1</sup>; <sup>1</sup>Los Alamos National Lab., Los Alamos, NM
- ThP 482 **Optimizing methods to extract metabolites from zebrafish tissue;** Michaela Schwaiger-haber<sup>1</sup>; Fuad J Naser<sup>1</sup>; Miriam Sindelar<sup>1</sup>; Jonathan L Spalding<sup>1</sup>; Gary J Patti<sup>1</sup>; <sup>1</sup>Washington University in St. Louis, St. Louis, MO
- ThP 488 **Comprehensive Studies of Drug-induced Stemness of Cancer Cells at Single-cell Level;** Mei Sun<sup>1</sup>; Xingxiu Chen<sup>1</sup>; Zhibo Yang<sup>1</sup>; <sup>1</sup>University of Oklahoma, Norman, OK
- ThP 493 **Comprehensive cell culture profiling of iPSC cell using LC-QTOFMS: Simultaneous analysis of SIM and Scan mode in a single run;** Takanari Hattori<sup>1</sup>; Toshiya Matsubara<sup>1</sup>; Tsuyoshi Nakanishi<sup>1</sup>; Jun Watanabe<sup>1</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan
- ThP 494 **Multi-omic analysis of macrophage and macrophage derived exosomes with Leishmania donovani infection;** Andrew P Kurland<sup>1</sup>; Vanessa Rubio<sup>1</sup>; Anna Gioseffi<sup>1</sup>; Peter Kima<sup>1</sup>; Timothy Garrett<sup>1</sup>; <sup>1</sup>University of Florida, Gainesville, FL
- ThP 508 **Assessing the Bioactivity of Environmental Surface Waters by Metabolomics Using Multiple Cell Lines;** Yang Yue<sup>1</sup>; Jonathan Mosley<sup>1</sup>; Paul Bradley<sup>2</sup>; Jenna Cavallin<sup>3</sup>; Daniel Villeneuve<sup>3</sup>; Gerald Ankley<sup>3</sup>; Drew Ekman<sup>1</sup>; Timothy Collette<sup>1</sup>; Qunicy Teng<sup>1</sup>; <sup>1</sup>U.S. Environmental Protection Agency, Athens, GA; <sup>2</sup>U.S. Geological Survey, Columbia, SC; <sup>3</sup>U.S. Environmental Protection Agency, Duluth, MN
- ThP 514 **MALDI-MS Proteotyping of Cutibacterium acnes;** Kanae Teramoto<sup>1</sup>; Tatsuki Okubo<sup>1</sup>; Yoshihiro Yamada<sup>1</sup>; Sadanori Sekiya<sup>1</sup>; Shinichi Iwamoto<sup>1</sup>; Koichi Tanaka<sup>1</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan



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- ThP 522 **HAMA: High-throughput Automated Muropeptide Analysis Framework for Revealing Composition of Bacterial Peptidoglycan;** Pin-rui Su<sup>1,2</sup>; Ya-Chen Hsu<sup>1</sup>; Hsin-Hsiang Chung<sup>1</sup>; Yun Lin<sup>1</sup>; Tsuey-Ching Yang<sup>3</sup>; Cheng-Chih Hsu<sup>1</sup>; <sup>1</sup>National Taiwan University, Taipei, Taiwan; <sup>2</sup>Erasmus MC, Rotterdam, Netherlands; <sup>3</sup>National Yang-Ming University, Taipei, Taiwan
- ThP 534 **Characterization of microorganisms by proteins and lipids MALDI-TOF fingerprints: case studies;** Vincent Guérineau<sup>1</sup>; Morgane Barthélemy<sup>1</sup>; Marceau Levasseur<sup>1</sup>; Téo Hébra<sup>1</sup>; Véronique Eparvier<sup>1</sup>; David Touboul<sup>1</sup>; <sup>1</sup>CNRS-ICSN, Gif Sur Yvette, France
- ThP 539 **Microbial Synthesis of a Novel Vitamin B9 Derivative and its Immunomodulatory Impact;** Abby J. Chiang<sup>1</sup>; Daniel Röth<sup>1</sup>; Anne E. Hall<sup>2</sup>; Gabriel B Gugiu<sup>1</sup>; James Versalovic<sup>2,3</sup>; Markus Kalkum<sup>1</sup>; <sup>1</sup>City of Hope, Duarte, CA; <sup>2</sup>Baylor College of Medicine, Houston, Texas; <sup>3</sup>Texas Children's Hospital, Houston, Texas
- ThP 541 **9.4 T FT-ICR Mass Spectrometer with Cluster Ion Source for Analysis of Molecular Nanocarbons;** Paul Dunk<sup>1</sup>; Yuri E. Corilo<sup>1</sup>; Christopher L. Hendrickson<sup>1</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL
- ThP 556 **High-sensitivity glycomic and proteomic profiling of limited biological samples using capillary zone electrophoresis-mass spectrometry;** Anne-Lise Marie<sup>1</sup>; Kendall Johnson<sup>1</sup>; Marcia Santos<sup>2</sup>; Somak Ray<sup>1</sup>; Antonius Koller<sup>1</sup>; David Frank<sup>3</sup>; Helen Gandler<sup>3</sup>; Shulin Lu<sup>3</sup>; John Tigges<sup>3</sup>; Ionita Ghiran<sup>3</sup>; Alexander R Ivanov<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Sciex, Brea, CA; <sup>3</sup>Harvard Medical School, Boston, MA
- ThP 560 **High-Sensitivity Analysis of Durgs in Ultra-Small Volumes Plasma Samples using Micro-Flow LC-MS/MS;** Davide Vecchiotti<sup>1</sup>; Mikaël Levi<sup>1</sup>; Hidetoshi Terada<sup>1</sup>; Jonathan Edwardsen<sup>2</sup>; Keiko Matsumoto<sup>1</sup>; Kyoko Watanabe<sup>1</sup>; Masami Tomita<sup>1</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>Shimadzu Scientific Instruments, Inc., Columbia, Maryland
- ThP 562 **In-syringe Electrokinetic Clean-up of Weakly Acidic Drugs in Biological Samples for Direct Injection Electrospray Ionization Mass Spectrometry;** Ibraam E Mikhail<sup>1,2,3</sup>; Masoomah Tehranirokh<sup>1,4</sup>; Andrew A Gooley<sup>1,4</sup>; Rosanne M Guijt<sup>1,5</sup>; Michael C Breadmore<sup>1,2</sup>; <sup>1</sup>ARC Training Centre for Portable Analytical Separation Technologies (ASTech), Hobart, Australia; <sup>2</sup>Australian Centre for Research on Separation Science (ACROSS), School of Physical Sciences (Chemistry), University of Tasmania, Hobart, Australia; <sup>3</sup>Department of Analytical Chemistry, Faculty of Pharmacy, Mansoura University, Mansoura, Egypt; <sup>4</sup>Trajan Scientific and Medical, Ringwood, Australia; <sup>5</sup>Centre for Regional and Rural Futures, Deakin University, Geelong, Australia
- ThP 563 **High-throughput proteome analysis using 50 cm long micro pillar array columns (μPACTM);** Jeff Op De Beeck<sup>1</sup>; Geert Van Raemdonck<sup>1</sup>; Paul Jacobs<sup>1</sup>; Gert Desmet<sup>2</sup>; Wim De Malsche<sup>2</sup>; Francis Impens<sup>3</sup>; Kris Gevaert<sup>3</sup>; <sup>1</sup>PharmaFluidics, Ghent, Belgium; <sup>2</sup>Vrije Universiteit Brussel, Brussels, Belgium; <sup>3</sup>VIB-UGent Center for Medical Biotechnology, Ghent, Belgium
- ThP 566 **Ultra-sensitive deep LC-MS proteomic profiling using ultra-low flow monolithic and porous-layer open tubular capillary columns;** Michal Gregus<sup>1</sup>; Antonius Koller<sup>1</sup>; Alexander R Ivanov<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA
- ThP 569 **Automation and Application of Magnetic Based Affinity Selection Screening for Targets of Retinoid X Receptor alpha (RXR?);** Ruth N Muchiri<sup>1</sup>; Jaewoo Choi<sup>1</sup>; Katherine A Carter<sup>1</sup>; Brett M Tyler<sup>1</sup>; Richard B. van Breemen<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, OR
- ThP 573 **Ozone-induced dissociation mass spectrometry as a new tool to determine the C=C double bond locations in natural products;** Ngoc Vu<sup>1</sup>; Sonja Knowles<sup>1</sup>; Nicholas Oberlies<sup>1</sup>; Qibin Zhang<sup>1,2</sup>; <sup>1</sup>UNC Greensboro, Greensboro, NC; <sup>2</sup>Center for Translational Biomedical Research, Kannapolis, NC
- ThP 578 **Using Ozone Induced Dissociation Mass Spectrometry (OzID-MS) for Natural Product Analysis: Pure Compound, Complex Extract, and In Situ;** Sonja L. Knowles<sup>1</sup>; Ngoc Vu<sup>1</sup>; Daniel A. Todd<sup>1</sup>; Huzefa A. Raja<sup>1</sup>; Antonis Rokas<sup>2</sup>; Qibin Zhang<sup>1,3</sup>; Nicholas H. Oberlies<sup>1</sup>; <sup>1</sup>University of North Carolina at Greensboro,



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- Greensboro, NC; <sup>2</sup>Vanderbilt University, Nashville, TN; <sup>3</sup>Center for Translational Biomedical Research, Kannapolis, NC
- ThP 580 **Bacteria Fight Club: Mapping Microbial Interactions for Drug Discovery;** Berkley Ellis<sup>1</sup>; Caleb N Fischer<sup>1</sup>; Brian O Bachmann<sup>1</sup>; John A. McLean<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN
- ThP 581 **Analysis of diterpenoids in *Tripterygium wilfordii* by supercritical fluid chromatography coupling tandem mass spectrometry;** Lingna Ke<sup>1</sup>; Ming Yuan<sup>2</sup>; Qing Fu<sup>1</sup>; Zhengwei Jia<sup>2</sup>; Yu Jin<sup>1</sup>; <sup>1</sup>East China University of Science and Technology, Shanghai, China; <sup>2</sup>Waters Technologies?Shanghai?Co?Ltd, Shanghai, China
- ThP 583 **Determination of Artemisinin and its precursors in *Artemisia annua* L using LC/MS/MS;** Huihua Ji<sup>1</sup>; Lowell Bush<sup>1</sup>; Neil Fannin<sup>1</sup>; <sup>1</sup>University of Kentucky, Lexington, KY
- ThP 585 **Using Dereplication for Targeted and Untargeted Re-Isolation of Fungal Secondary Metabolites;** Allison J. Wright<sup>1</sup>; Sonja L. Knowles<sup>1</sup>; Huzefa A. Raja<sup>1</sup>; Nicholas H. Oberlies<sup>1</sup>; <sup>1</sup>University of North Carolina at Greensboro, Greensboro, NC
- ThP 591 **The Effect of G-quadruplexes on the Stability of Adjacent DNA Domains Studied by Temperature-controlled nanoESI-MS;** Adam Pruška<sup>1</sup>; Adrien Marchand<sup>1</sup>; Renato Zenobi<sup>1</sup>; <sup>1</sup>ETH Zurich, Zurich, Switzerland
- ThP 602 **Investigation of matrix conditions for nucleic acid analysis in positive ion detection using a linear benchtop MALDI-TOFMS;** Shuichi Nakaya<sup>1</sup>; Akihiro Kunisawa<sup>2</sup>; Zenzaburo Tozuka<sup>2</sup>; Yuzo Yamazaki<sup>1</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>Shimadzu Analytical Innovation Research Laboratory, Osaka University, Suita, Japan
- ThP 607 **Simultaneous quantification of dA-Ap and dG-Ap interstrand cross-links in cellular and tissue DNA;** Su Guo<sup>1</sup>; Jiapeng Leng<sup>1</sup>; Yinsheng Wang<sup>1</sup>; <sup>1</sup>UC Riverside, Riverside
- ThP 615 **Combined Density Functional and Statistical Analyses of Doubly Protonated Tryptic Peptide Series;** Shanshan Guan<sup>1</sup>; Benjamin J Bythell<sup>1</sup>; <sup>1</sup>University of Missouri, St. Louis, St. Louis, MO
- ThP 625 **High Resolution - Mass Spectrometry Cellular Thermal Shift Assay (HR-MS-CETSA)- impact of phosphorylation on thermal protein stability;** Yan Ting Lim<sup>1</sup>; Tianyun Zhao<sup>2</sup>; Wint Wint Phoo<sup>1</sup>; Lingyun Dai<sup>2</sup>; Loo Chien Wang<sup>1</sup>; Liyan Chen<sup>1</sup>; Par Nordlund<sup>1,2,3</sup>; Radoslaw Sobota<sup>1</sup>; <sup>1</sup>Institute of Molecular and Cell Biology Agency for Science, Technology and Research (A\*STAR), Singapore, Singapore; <sup>2</sup>School of Biological Sciences, Nanyang Technological University, Singapore, Singapore, Singapore; <sup>3</sup>Karolinska Institutet, Department of Oncology-Pathology, Stockholm, Sweden
- ThP 633 **Integrated structural proteomics and dynamics of a solid-body organism by combined XLMS, solvent accessible surface modification and QconCAT;** Yeva Mirzakhanyan<sup>1</sup>; Paul Gershon<sup>1</sup>; <sup>1</sup>UC-Irvine, Irvine, CA
- ThP 634 **Analysis of Human Nuclear Protein Complexes by Quantitative Mass Spectrometry Profiling;** Katelyn E. Connelly<sup>1</sup>; Victoria Hedrick<sup>2</sup>; Tiago J. P. Sobreira<sup>2</sup>; Emily C. Dykhuizen<sup>1</sup>; Uma K. Aryal<sup>2</sup>; <sup>1</sup>Department of Medicinal Chemistry and Molecular Pharmacology Purdue University, West Lafayette, IN; <sup>2</sup>Purdue Proteomics Facility, Bindley Bioscience Center, West Lafayette, IN
- ThP 639 **Structural characterization of ternary complexes for selective protein degradation by hydrogen-deuterium exchange mass spectrometry;** Jing Li<sup>1</sup>; Aaron Balog<sup>1</sup>; Louis Lombardo<sup>1</sup>; John Newitt<sup>1</sup>; Mark Witmer<sup>1</sup>; Guodong Chen<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb, Princeton, NJ
- ThP 642 **Coupling FPOP with IM-MS for detailed structural characterization of the native ensemble of cytochrome c;** Emily E Chea<sup>1</sup>; Daniel Deredge<sup>1</sup>; Lisa M Jones<sup>1</sup>; <sup>1</sup>University of Maryland, Baltimore- School of Pharmacy, Baltimore, MD
- ThP 648 **Assessing the Comparability of Ion Mobility Mass Spectrometry to Measure Collision Cross Section Distributions for Protein Standards;** Aidan P France<sup>1</sup>; Lukasz Migas<sup>2</sup>; Bruno Bellina<sup>2</sup>; Eleanor Sinclair<sup>2</sup>;



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- ThP 655 Perdita E. Barran<sup>2</sup>; <sup>1</sup>University of Manchester, Manchester, United Kingdom; <sup>2</sup>Manchester Institute of Biotechnology, University of Manchester, United Kingdom  
**Co-localization of CD147 with oncogenic proteins confers drug-resistant phenotype in breast cancer stem cells;** Sohyun Kim<sup>1</sup>; Yuri Seo<sup>1</sup>; Hyeryeon Jung<sup>1</sup>; Jieun Jung<sup>2</sup>; Yeojin Jung<sup>2</sup>; Kristine M Kim<sup>2</sup>; Eugene C Yi<sup>1</sup>; <sup>1</sup>Department of Molecular Medicine and Biopharmaceutical Sciences, Graduate School of Convergence Science and Technology, Seoul National University, Seoul, South Korea; <sup>2</sup>College of Biomedical Science, Kangwon National University, Seoul, South Korea
- ThP 663 **Intact and Subunit Mass Analysis Using Native Ion Exchange Chromatography Coupled to an Orbitrap Mass Spectrometer;** Qian Liu<sup>1</sup>; Stephane Houel<sup>1</sup>; Hao Zhang<sup>1</sup>; Alla Polozova<sup>1</sup>; <sup>1</sup>Amgen Inc., Cambridge, MA
- ThP 679 **Phosphonate-modified core-shell structured Fe<sub>3</sub>O<sub>4</sub>-SiO<sub>2</sub> nanoparticles: synthesis, characterization and application to the enrichment of phosphopeptides;** Qingshi Meng<sup>1</sup>; Xiaohui Feng<sup>1</sup>; Xiangfang Tang<sup>1</sup>; Hongfu Zhang<sup>1</sup>; <sup>1</sup>Institute of Animal Sciences, CAAS, Beijing, China
- ThP 680 **The Acetylation of Lysine-376 of G3BP1 Regulates RNA Binding and Stress Granule Dynamics;** Jing Chen<sup>1</sup>; Jozsef Gal<sup>2</sup>; Duck-Young Na<sup>2</sup>; Laura Tichacek<sup>2</sup>; Kelly R Barnett<sup>2</sup>; Haining Zhu<sup>2,3</sup>; <sup>1</sup>University of Kentucky, Lexington, KY; <sup>2</sup>University of Kentucky, Lexington, Kentucky; <sup>3</sup>Lexington VA Medical Center, Research & Development, Lexington, Kentucky
- ThP 683 **LC-MS analysis of bound sulfane sulfur in hypoxic endothelial cells;** Xinggwei Shen<sup>1</sup>; Christopher B. Pattillo B. Pattillo<sup>1</sup>; Hyung W. Nam<sup>1</sup>; Christopher G. Kevil<sup>1</sup>; <sup>1</sup>LSU Health-shreveport, Shreveport, LA
- ThP 692 **Ubiquitinome dynamics upon proteasome modulation;** Jeroen Demmers; Erasmus University Medical Center, Rotterdam, Netherlands
- ThP 693 **Exploring the Open Proteome: Proteomics Open Search Analysis with PTM-Shepherd;** Daniel J Geiszler<sup>1</sup>; Andy T. Kong<sup>1</sup>; Dmitry M Avtonomov<sup>1</sup>; Felipe Da Veiga Leprevost<sup>1</sup>; Hui-Yin Chang<sup>1</sup>; Alexey I. Nesvizhskii<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI
- ThP 696 **Identification and functional characterizations of novel proteins promoting ?-N-demethylation;** David Bade<sup>1</sup>; Lin Li<sup>1</sup>; Xiaoxia Dai<sup>1</sup>; Yinsheng Wang<sup>1</sup>; <sup>1</sup>UC Riverside, Riverside, CA
- ThP 724 **Detection of aberrant proteoforms from alternative splicing events in tandem mass tagged proteomic datasets;** Daniel Roeth<sup>1</sup>; Meiling Jin<sup>1</sup>; Yiming Wu<sup>1</sup>; Lili Wang<sup>1</sup>; Markus Kalkum<sup>1</sup>; <sup>1</sup>City of Hope, Duarte, CA
- ThP 733 **Cellular responses of breast cancer cell line to anti-cancer medicinal compounds from ginger root;** Parvin Mirzaei<sup>1</sup>; Luke Brown<sup>2</sup>; Jaicee Tudman<sup>2</sup>; Adam Reinhart<sup>2</sup>; Masoud Zabet Moghaddam<sup>1</sup>; <sup>1</sup>Texas Tech University, Lubbock, TX; <sup>2</sup>Wayland Baptist University, Plainview, TX
- ThP 736 **Optimizing mass spectrometry proteomic analysis of isolated brain myeloid cells;** Sruti Rayaprolu<sup>1,2</sup>; Tianwen Gao<sup>2,3</sup>; Hailian Xiao<sup>1,2</sup>; Supriya Ramesha<sup>1,2</sup>; Duc M Duong<sup>1,4</sup>; Eric B. Dammer<sup>1,4</sup>; James J. Lah<sup>1,2</sup>; Allan I. Levey<sup>1,2</sup>; Nicholas Seyfried<sup>1,4</sup>; Srikant Rangaraju<sup>1,2</sup>; <sup>1</sup>Center for Neurodegenerative Diseases, Emory School of Medicine, Atlanta, GA; <sup>2</sup>Department of Neurology, Emory University, Atlanta, GA; <sup>3</sup>Emory University - Center of Neurodegenerative Diseases, Atlanta, GA; <sup>4</sup>Department of Biochemistry, Emory University, Atlanta, GA
- ThP 739 **Use of the Cysteine proteome to increase coverage in quantitative proteomics and assess reversible cysteine modifications in T-cell signaling;** Martin R. Larsen<sup>1</sup>; Taewook Kang<sup>1</sup>; Arkadiusz Nawrocki<sup>1</sup>; Komal K. Mandal<sup>1</sup>; Muhammad Tahir<sup>1</sup>; <sup>1</sup>Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense, Denmark
- ThP 740 **IonStar.Mine: Extending Quantitative Depth of IonStar by High-Resolution MS1-Based Feature Matching;** Shichen Shen<sup>1</sup>; Shuo Qian<sup>1</sup>; Min Ma<sup>2</sup>; Ming Zhang<sup>1</sup>; Jun Qu<sup>1</sup>; <sup>1</sup>University at Buffalo, Buffalo, NY; <sup>2</sup>Roswell Park Comprehensive Cancer Center, Buffalo, NY
- ThP 768 **High sensitivity LC-HRMS method for retinoids quantification;** Laurent Laboureur<sup>1,2</sup>; Elaine Shanling Ho<sup>1,2</sup>; Ian A. Blair<sup>1,2</sup>; Clementina Mesaros<sup>1,2</sup>; <sup>1</sup>Penn SRP Center and Center of Excellence in Environmental



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ThP 770

**Improved Sensitivity for Bioanalysis of Pyrrolobenzodiazepine Dimers Using Microflow HPLC Coupled with Tandem Mass Spectrometry; Rolf Kern; SCIEX, Redwood Shores, CA**