Oral Presentations

Wednesday, June 7

8:50-9:10 AM, 500 Ballroom Level 1
The Advantages of Using MS/MS\textsuperscript{ALL} with SWATH\textsuperscript{®} Acquisition for Confident Compound Identification
Paul C. Winkler; Craig Butt; April Quinn-Paquet
SCIEX

10:10-10:30 AM, 500 Ballroom Level 1
Identification of Major Chemical Constituents in Momordica charantia Using Liquid Chromatography-Mass Spectrometry and Its Lipase Inhibitory Activity
Joydeb Chanda\textsuperscript{1}; Pulok Kumar Mukherjee\textsuperscript{2}; Sayan Biswas\textsuperscript{2}; Suvodip Banerjee\textsuperscript{2}; Amit Kar\textsuperscript{2}; Faraz Rashid\textsuperscript{2}; Dipanakar Malakar\textsuperscript{2}; Manoj Pillai\textsuperscript{3}
\textsuperscript{1}School of Natural Product Studies, India; \textsuperscript{2}School of Natural Product Studies, Department of Pharmaceutical Technology, Jadavpur University, India; \textsuperscript{3}SCIEX India

2:30-2:50 PM, Sagamore 4 Level 2
Letting Ozone-induced Dissociation Out of the Box: A Modular, Platform-Independent System for Implementation in Diverse Lipidomics Workflows
Berwyck L. J. Poad\textsuperscript{1}; Stephen J. Blanksby\textsuperscript{1}; David L. Marshall\textsuperscript{2}; Reuben S. Young\textsuperscript{1}; Todd W. Mitchell\textsuperscript{2}; J. Larry Campbell\textsuperscript{2}; Eva Duchoslav\textsuperscript{3}; Martin R. Green\textsuperscript{4}; Jayne Kirk\textsuperscript{4}; Nick Tomczyk\textsuperscript{5}; Shane R. Ellis\textsuperscript{6}; Martin R. L. Paine\textsuperscript{2}; Ron M. A. Heeren\textsuperscript{7}
\textsuperscript{1}Queensland University of Technology, Australia; \textsuperscript{2}University of Wollongong, Australia; \textsuperscript{3}SCIEX; \textsuperscript{4}Waters Corporation; \textsuperscript{5}Maastricht Multi-Modal Molecular Imaging (M4I) Institute, Maastricht University, Netherlands

Poster Presentations

All posters are located in the Posters/Exhibit Hall; Odd-number posters present 10:30 AM-1:00 PM; Even-number posters present 12:00-2:30 PM

Monday, June 5

#018
Robust and Sensitive Workflow for Qualitative and Quantitative Analysis of Intact Monoclonal Antibodies Using Microflow LC and TripleTOF\textsuperscript{®} Mass Spectrometry
Gavin Fischer; Susan Darling
SCIEX

#020
Charge Heterogeneity Analysis of Intact Monoclonal Antibodies Using CESI-MS
Esme Candish\textsuperscript{1}; Christopher Loesener\textsuperscript{2}; Stephen J. Lock\textsuperscript{2}; Olga Friesen\textsuperscript{3}; Elaine Stephens\textsuperscript{1}; Jason C. Rouse\textsuperscript{4}; Bryan Fonslow\textsuperscript{1}
\textsuperscript{1}SCIEX; \textsuperscript{2}SCIEX Germany; \textsuperscript{3}SCIEX United Kingdom; \textsuperscript{4}Biotherapeutics Pharm. Sci., Pfizer Inc.

#075
N-glycosylation Analysis of mAbs by CESI-MS at the Glycopeptide and Released Glycan Levels
Jenny Albanese\textsuperscript{1}; Marton Szigeti\textsuperscript{2}; Bryan Fonslow\textsuperscript{1}; Andreas Guttmann\textsuperscript{1}; Edna Betgovargez\textsuperscript{1}
\textsuperscript{1}SCIEX; \textsuperscript{2}University of Debrecen, Hungary

#081
Automated and Rapid Characterization of Low-Molecular-Weight Heparin Oligosaccharides Using TripleTOF\textsuperscript{®} 5600 Mass Spectrometer with SimGlycan Software
Ningombam Sanjib Meitei\textsuperscript{1, 2}; Rajesh Pujari\textsuperscript{3}; Arun Apte\textsuperscript{3}; Annu Uppal\textsuperscript{3}
\textsuperscript{1}PREMIER Biosoft, India; \textsuperscript{2}PREMIER Biosoft; \textsuperscript{3}SCIEX India
Poster Presentations
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Monday, June 5 (continued)

#111
Clinical Applications by Direct Coupling of Bio-Compatible SPME Devices to MS via Open-Port Probe Sampling Interface
Marcos Tascon¹; German Gomez-Rios¹; Chang Liu²; Anna Roszkowska¹; Nikita Looby¹; Nathaly Reyes Garces¹; Don W. Arnold²; Tom Covey²; Barbara Bojko¹,³; Janusz Pawliszyn¹
¹Department of Chemistry, University of Waterloo; ²SCIEX; ³Department of Pharmacodynamics and Molecular Pharmacology, Faculty of Pharmacy, Nicolaus Copernicus University, Poland

#147
An Open Port Sampling Interface for High-Throughput SPME-MS/MS Analysis of in vitro ADME Samples
John Janiszewski¹; Brendon Kapinos¹; Sara Smith²; Craig Aurand²; Chang Liu³; Tom Covey³; German Augusto Gomez-Rios⁴
¹Pfizer Inc.; ²MilliporeSigma; ³SCIEX; ⁴University of Waterloo

#228
Using Differential Mobility Spectrometry to Separate Chiral Compounds: Amphetamines
J. Larry Campbell; J.C. Yves LeBlanc; Chang Liu
SCIEX

#313
Protein Identification without Peptide Identification
Jamie Sherman; Stephen Tate
SCIEX

#350
Open-Port Probe Sampling Interface for the Direct Coupling of Solid-Phase Microextraction to Atmospheric Pressure Ionization Mass Spectrometry
Chang Liu¹; Germán Gómez-Ríos²; Marcos Tascon³; Bradley B. Schneider¹; Nathaly Reyes-Garcés²; Don W. Arnold¹; Thomas R. Covey¹; Janusz Pawliszyn³
¹SCIEX; ²University of Waterloo

#372
The Use of SelexION® Technology to Increase Sensitivity for Trace Level Analysis of Small Molecules
Christopher Borton¹; Paul C. Winkler¹; Jay Jones³
¹SCIEX; ³BASF

#423
Robust and High Throughput Lipid Profiling in Dried Blood Spot Samples Using Automated FIA MSMSAll Technique
Kuldeep Ravivanshi¹; Narinder Sahni²; Akanksha Singh³; Dipanakar Malakar²; Manoj Pillai³
¹Lipomic Healthcare Pvt. Ltd, India; ²Jawaharlal Nehru University, India; ³SCIEX India

#484
Evaluation of High Speed, High Resolution Data Independent Acquisition for Simultaneous Identification and Quantitative Metabolomic Flux Analysis
Loren Olson¹; Emile Plise²; Baljit Ubhi³
¹SCIEX; ²Genentech, Inc.

#486
Detection and Quantitation of Sugar Phosphate Metabolite Markers in Femto Molar Concentration Using 6500+ QTRAP® LCMS/MS System
Manoj Pillai; Dipankar Malakar; Faraz Rashid
SCIEX India
**Poster Presentations**

Poster Presentations
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**Monday, June 5 (continued)**

#525
Designing Targeted Detection of Peptides in Complex Matrices Combining the MIDAS™ Workflow with the Skyline Software
Jenny Albanese1; Christie Hunter1; Kaipo Tamura2; Brendan MacLean3
1SCIEX; 2William S. Noble Department of Genome Sciences, University of Washington; 3UW Medicine

#528
Scout-MRM Simplifies Targeted Assay Development from Public Proteomic Dataset: A Yeast Proteome Case Study
Lény Garcia1; Romain Carrier1; Eric Testet2; Pathy Laquel2; François Doignon3; Yves LeBlanc4; Ayciriex Sophie4; Jérôme Lemoine5
1Institut des Sciences Analytiques, Université de Lyon, France; 2Institut Polytechnique de Bordeaux, France; 3Université de Bordeaux, France; 4SCIEX; 5Université de Lyon, Villeurbanne

**Tuesday, June 6**

#062
Use Information Independent SWATH® Acquisition for Biotherapeutic Peptide Mapping
Ji Luo
SCIEX China

#063
BiopharmaView™ Software as a Robust Tool for Automated Quantitation of Oxidation Sites in Monoclonal Antibody Characterization
Kerstin Pohl1; Annu Uppal2; Amandine Boudreau3
1SCIEX Germany; 2SCIEX India; 3SCIEX

#065
HRAMS Monitoring of In-Vivo Protein Biotransformation’s: Quantitative Determination of Trastuzumab and Deamidation Products in Human Plasma by MRM® and SWATH® Acquisition
Jason Causon1; Kees Bronsema2; Nico Van De Merbel2; Edwin Hooijschuur2; Martijn Hlihorst2; Milia Neffling2; Neil Walsh1
1SCIEX United Kingdom; 2PRA HealthSciences, Netherlands

#073
Mapping the Effects of UV Irradiation on Monoclonal Antibody Drugs
J. Larry Campbell1; Chris Lock1; Brendon Seale1,2; J.C. Yves LeBlanc1; Suya Liu1; Xu Guo1; Wen Jin1; Michael Sasges3; Michelle Gabriel3; Mark Schofield4; Marc Aucoin5; Emma Dare6
1SCIEX; 2University of Toronto; 3Trojan Technologies; 4Pall Corporation; 5University of Waterloo

#078
Determination of Released Payload Species of Antibody Drug Conjugates with Noncleavable Linkers by High Resolution Mass Spectrometry and MetabolitePilot™ Software
Ian Moore; Yuan-Qing Xia
SCIEX

#145
The Advantages of Using an MRM® Acquisition for Increased Sensitivity for Targeted Analysis Using a QTOF Instrument
Paul C. Winkler; K.C. Hyland; Christopher Borton
SCIEX
Poster Presentations

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Tuesday, June 6 (continued)

#147
Quantitation of Triptorelin in Rat Plasma Using Triple Quadrupole Mass Spectrometry
Ting Liu; Lin Zhu; Wenhai Jin; Xiongwei Yang; Jingsheng Zhang; Jifeng Deng
SCIEX China

#156
Comparison of Combining Quantitative with Qualitative Met ID Analysis in the QTRAP® 6500 and TripleTOF® 5600 Mass Spectrometer
Minli Zhang1; Keith J. Goodman2; Diane L. Nabb1; Heather Peterson1; John M. Hevko2
1DuPont; 2SCIEX

#168
Scanning-SWATH® Acquisition for Pesticide Analysis and Quantitation
Nic Bloomfield; J.C. Yves LeBlanc; Gordana Ivosev; Ian Tremble; Jamie Sherman; Andre Schreiber
SCIEX

#186
Analyzing Spent Grains as a Sustainable Source of Feed
Liesl Krone1; BJ Bench2; Manju Bala3; Andre Schreiber4; Jennifer Krone5; Oscar Cabrices6
1Granbury High School; 2Food Safety and Research Laboratory, Tyson Foods; 3CPS, PLLC; 4SCIEX Germany; 5SCIEX; 6GERSTEL, Inc.

#201
Sensitive and Specific Allergen Screening Analysis Using LC-MS/MS
Paul C. Winkler; Hua-Fen Liu; Christopher Borton; Leesun New
SCIEX

#218
Quantitation of THC and Metabolites in Whole Blood by LC-MS/MS for Per Se Law Testing
Diana Tran1; Xiang He1; Tracy Blethen1; Kevin Kopp2; Alexandre Wang1; Hua-Fen Liu1
1SCIEX; 2UTAK Laboratories Inc.

#221
Drug Analysis in Urine by Thermal Desorption and Pyrolysis Combined with DART-MS (TDP/DART-MS)
Hiroko Abe1; Chikako Takei2; Yasuo Shida3; Motoshi Sakakura3; Teruhisa Shiotani2; Kayako Suga4; Daisuke Yajima1; Hirotarō Iwase5,6
1University of Chiba, Japan; 2BioChromato, Inc., Japan; 3AMR Inc., Japan; 4SCIEX Japan; 5University of Tokyo, Japan

#223
A Novel Liquid Chromatography Tandem Mass Spectrometry Method Detection of Deinagkistrodon acutus venom in vivo
Hangqi Li1; Jia Lin1; Chao Zhang2; Peibin Qin2; Huaidong Yu2
1Institute of Forensic Science of Fujian Public Security Department, China; 2SCIEX Asia Pacific Application Support Center, China

#376
Enhanced Ion Charging Effect of m-Nitro Benzyl Alcohol (m-NBA) on Protein and Peptides Characterization
Dipankar Malakar; Faraz Rashid; Manoj Pillai
SCIEX INDIA

#392
Run, MS, Run! Increasing System Robustness with Ion Control
Brent Lefebvre; Yang Kang; Mauro Aiello; Bradley B. Schneider; J.C. Yves LeBlanc7
SCIEX
**Poster Presentations**

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**Tuesday, June 6 (continued)**

#448

Electromagnetic Mixer for Highly Efficient, Automated Sample Preparation
Chang Liu; Don W. Arnold; Thomas R. Covey
SCIEX

#484

Authentication of Two Different Types of Fish Oils by Qualitative Lipid Profiling Using Semi-Targeted Approach on QTRAP® Platforms
Niladri Sekhar Chatterjee¹; Akanksha Singh²; Vishnu KV¹; Ajeeshkumar K K¹; Anandan R¹; Ashok Kumar¹; Suseela Mathew¹; Manoj Pillai²
¹ICAR-Central Institute of Fisheries Technology, India; ²SCIEX India

#648

Standardizing and Harmonizing Multiple TripleTOF® Systems for DDA and DIA Using a Dedicated Performance Kit
Nicholas Morrice¹; Tom Knapman¹; Hunter Christie³; Robert Graham³; Julie Brazzatti³; Anthony Whetton⁷
¹SCIEX United Kingdom; ²SCIEX; ³University of Manchester, United Kingdom

#649

High Throughput Microflow LC-MS/MS for High Sensitivity Peptide Quantitation in Targeted Assays
Remco van Soest¹; Christie Hunter¹; Morty Razavi²
¹SCIEX; ²SISCAPA Assay Technologies

#720

Analytical Data Longevity and Management for Regulatory Compliance Using AnIML Format and Cloud Technologies
John Gibbons¹; Viktor N. Iassinskii¹; Burkhard Schaefer²
¹SCIEX; ²BSSN Software GmbH, Germany

**Wednesday, June 7**

#065

Profiling Biochemical Individuality: Human Personal Omics Profiling (hPOP)
Sara Ahadi¹; Hannes Roest¹; Liang Liang¹; Christie Hunter²; Mike Snyder³
¹Stanford School of Medicine; ²SCIEX

#068

Analysis of m/z Distribution of Tryptic Peptides in Various Types Biological Samples, Supporting Generic DIA Strategies
Faraz Rashid; Manoj Pillai; Dipankar Malakar
SCIEX India

#087

Universal Data-Independent LC-MS/MS Workflow for Host Cell Protein Characterization and Quantification in Biopharmaceutical Product Purification Process
Lei Xiong¹; Yihan Li¹; Stephen Tate¹; Todd Stawicki¹; Edita Botonjic-Sehic²; Mark Schofield³; Vincent Ravault⁴; Sean McCarthy⁴; Hua-Fen Liu¹
¹SCIEX; ²Pall Corporation; ³Pall Corporation France

#100

Fast and Comprehensive Detection and Characterization of Cyclic Peptide Metabolites Using Software-Aided Data Processing Tools
Ming Yao¹; Eva Duchoslav²; Li Ma¹; Silvi Chacko¹; Mingshe Zhu¹
¹Bristol-Myers Squibb; ²SCIEX

#104

A Metabolite ID Workflow on a Small Footprint Benchtop Q-TOF Mass Spectrometer with Automated Software Structure Generation
Shaokun Pang; Ian Moore
SCIEX
Poster Presentations
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Wednesday, June 7 (continued)

#106
High-Throughput and Automated Software Workflow Strategies for Small Molecule Identification and Characterization Using a High Resolution Q-TOF Mass Spectrometer
Alina Dindyal-Popescu; Iris Shek; Mohammed Jooyandeh; Ian Moore; Eva Duchoslav
SCIEX

#107
The Application of Research Grade MetabolitePilot™ Software for the Determination of Exenatide Catabolites Using HRAM with SWATH® Acquisition
Jeff Plomley¹; Yi Zhang²; Eva Duchoslav²; Daniel Villeneuve¹; Kevork Mekhssian¹; Anahita Keyhani¹
¹Algorithme Pharma an Altasciences Company; ²SCIEX

#135
Determination of Trace Levels of Microcystins in Aqueous Samples by Direct Injection LC-MS/MS
Paul C. Winkler; Craig Butt; April Quinn-Paquet
SCIEX

#415
Enantiomer Identification in Eicosanoids Using Hydrogen-Deuterium Exchange (HDX) - Electron Induced Dissociation (EID) Mass Spectrometry
Takashi Baba; J. Larry Campbell; J.C. Yves LeBlanc; Paul RS Baker
SCIEX

#469
Metabolic Determination of Acetaminophen in Down Syndrome Disease Research Using Targeted Mass Spectrometry
Melanie Juba¹; Christina Iverson²; Olivia Iverson³; Jeffrey Miller¹; Baljit Ubhi¹
¹SCIEX; ²Algonquin Regional High School; ³Boston University

#483
Simultaneous Determination of Key Glycolysis and Tricarboxylic Acid Cycle Intermediates in Fluxomics Studies by DMS-LC/MS/MS
Mary A Piotrowski¹; Darren Dumlao¹; Julie Keefe¹; John Janiszewski¹; Richard Kibbey²; Tiago Alves³; Bradley B. Schneider²; Chang Liu³; J. Larry Campbell³; Paul RS Baker³; Yves LeBlanc³; Keith J. Goodman³; Tanya Gamble³
¹Pfizer Inc.; ²Yale University; ³SCIEX

#575
SWATH® Data Independent Acquisition Strategies for Ultimate Confidence in Peptide Mapping and Post-Translational Modifications Quantitation for Biotherapeutics Characterization
Sibylle Heidelberger¹; Annu Uppal²
¹SCIEX; ²SCIEX India

#633
Development of an Affinity Capture-LC-MS/MS Assay for the Quantitation of Adalimumab in Human Plasma Using BioBA Sample Preparation Kit
Jean-François Dupuis¹; Kevork Mekhssian¹; Ian Moore²; Anahita Keyhani¹
¹Altasciences; ²SCIEX

#642
Targeted, Site-specific Quantitation of N- and O-glycopeptides of Biologics Using 18O-labeling and Product Ion Based Mass Spectrometry
Jandhyam Srikanth¹; Rathinasamy Agalyadevi¹; Ponnusamy Babu¹; Annu Uppal²
¹National Centre for Biological Sciences, Glycomics and Glycoproteomics & Biologics Characterization Facility, India; ²SCIEX India
Poster Presentations
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12:00-2:30 PM

Wednesday, June 7 (continued)

#657
Improved Sensitivity for LC-MS Quantitation of Biologics in Plasma Using Trap-and-Elute MicroLC-MS
Remco van Soest; Khatereh Motamedchaboki; Sibylle Heidelberger; Ian Moore
SCIEX

Thursday, June 8

#114
Targeted Sphingolipid Profiling of Tumor and Plasma Samples in Murine Lung Carcinoma Model Revealing the
Mechanism of Doxorubicin
Ujjaini Dasgupta1; Nihal Medatwal2; Avinash Bajaj2; Dipanakar Malakar2; Manoj Pillai2; Sandeep Kumar2
1Amity Institute of Integrative Sciences & Health, Amity University, India; 2Regional Center for Biotechnology, India; 3SCIEX India

#167
The Analysis of Environmental Samples Using High Resolution Mass Spectrometry to Identify Novel PFAS
Compounds
Paul Č. Winkler; Simon Roberts; Craig Butt; Christopher Burton
SCIEX

#191
Fast Space Charge Simulations: Simulation of Ion – Ion and Background Gas Interaction in a Linear Quardrupole
Walter Wissdorf1; Hendrik Kersten1; Thorsten Benter1; Tom Covey2; Jim Hager2; Bradley B. Schneider2
1Bergische Universität Wuppertal, NRW; 2SCIEX

#192
Effects of Chemical Dynamics and Clustering Reactions of Chemical Modifiers with Analyte Ions in Differential
Mobility Spectrometry (DMS)
Florian Stappert1; Marco Thinius1; Hendrik Kersten1; Walter Wissdorf1; Tom Covey2; Bradley B. Schneider2; Jim Hager2; Thorsten Benter1
1Bergische Universität Wuppertal, NRW; 2SCIEX

#246
Using SWATH® Acquisition with Differential Ion Mobility for Accurate Mass Flux Analysis
Tiago Cardoso Alves1; Keith J. Goodman2; Sabu George3; Abhishek Jha4; Rebecca L. Cardone5; Richard G. Kibbey4
1Yale University; 2SCIEX; 3Elucidata; 4Yale University

#254
Monitoring Critical Quality Attributes Supporting Development of Biopharmaceuticals
Sean McCarthy; Sibylle Heidelberger
SCIEX

#255
Mass Accuracy and Robustness of Intact mAb on the X500B Benchtop Quadrupole-Time-Of-Flight Instrument
Fan Zhang1; Chris Nortcliffe2; Sibylle Heidelberger1
1SCIEX; 2SCIEX United Kingdom

#392
Mitigating Fragmentation of Peptides with Controlled Clustering
J.C. Yves LeBlanc1; Brendon Seale1,2; Bradley B. Schneider1; Aaron Wheeler2
1SCIEX; 2University of Toronto

#449
Structural Characterization of Bioactive Fatty Acid Isomers Using Liquid Chromatography–Differential Mobility
Spectrometry and Electron-Induced Dissociation Mass Spectrometry (LC-DMS-EID)
Kazutaka Ikeda1,2; Shuh Yasuda1; Yuuya Seno1; Makoto Anai1,2,3; J. Larry Campbell; J.C. Yves LeBlanc4; Paul RS Baker5; Takashi Baba4
1RIKEN Center for Integrative Medical Sciences, Japan; 2Yokohama City University, Japan; 3Keio University, Japan; 4SCIEX
Poster Presentations

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Thursday, June 8 (continued)

#459
Development of an HILIC Based LC-MS/MS for High-Throughput Targeted Lipidomics
Junhua Wang; Mackenzie Pearson; Paul RS Baker
SCIEX

#462
Dysregulated Lipid Profiles of Non-Alcoholic Fatty Liver Disease (NAFLD)
Timothy J Garrett¹; Rainey E Patterson²; Baljit Ubhi³; Ken Cusi¹
¹University of Florida; ²Eastman Chemical Company; ³SCIEX

#497
A Novel Labeled Metabolomics Workflow Applying Isotope Ratio Outlier Analysis (IROA) and SWATH® Acquisition for Unambiguous Compound Identification
Baljit Ubhi¹; Felice de Jong²; Chris Beecher²,³
¹SCIEX; ²IROA Technologies; ³University of Florida

#499
A Simplified, Integrated Solution for Untargeted Metabolomics
Baljit Ubhi¹; Ranjan Perera²; Matthew Skaley¹; Timothy J. Garrett³
¹SCIEX; ²Sanford Burnham Prebys Medical Discovery Institute; ³University of Florida

#507
Benefits of SWATH® Acquisition, a DIA Technique over Traditional Data Dependent Analysis for High Resolution Untargeted Metabolomics Applications
Hector Gallart-Ayala¹; Zuzana Demianova²; Cyrus Papan²; Joerg Dojahn²; Baljit K. Ubhi³
¹SCIEX Spain; ²SCIEX Germany; ³SCIEX

#591
Protein Disulfide Bond Characterization with DMS and ECD
J.C. Yves LeBlanc¹; Brendon Seale¹, ²; Lyle Burton¹; Takashi Baba¹
¹SCIEX; ²University of Toronto

#685
Streamlining PCT-HD for Tissue Biopsy Samples: Better Digestion in a Shorter Time
Vera S. Gross¹; Keith Ashman²; Peter Hains²; Alexander Lazarev¹
¹Pressure BioSciences; ²SCIEX; ³Children’s Medical Research Institute, Australia

#700
Differential Mobility Separation with SCIEX SelexION® Technology – A Novel Technique for the Bioanalysis of Poor Fragmenting Molecules Like Valproic Acid
Jeyan Albert¹; Anoop Kumar¹; Manoj Pillai¹; Peeyush Jain⁴; Naveen Dubey⁵; Sandeep Sharma⁵
¹SCIEX India; ²Jubilant Generics Ltd, India