



Welcome to the 63rd ASMS Conference on Mass Spectrometry and Allied Topics. Conference program activities and exhibit booths are in America's Center. Corporate Member hospitality suites are located in the Renaissance Grand Hotel.

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- Zef Scientific, Inc.

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*Titles in the following sections are provided by authors. The complete abstracts are available online: [www.asms.org](http://www.asms.org)*

*The PDF document of proceedings submissions for orals and posters may be viewed online one day after presentation at the conference.*

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## GENERAL INFORMATION

**REGISTRATION** is open 10:00 am - 8:00 pm on Sunday and 7:30 am - 5:00 pm on Monday through Thursday.

### ATTENTION UNDERGRADUATE STUDENTS AND FIRST TIME (AT ASMS) GRADUATE STUDENTS

4:00 - 4:45 pm, Sunday, Ballroom 220/221

**Plan Your Strategy: What to See and Do at ASMS**

### SUNDAY TUTORIAL SESSION, 5:00 - 6:30 PM

Hall 5, level 1



5:00 - 5:45 pm  
**Statistical Experimental Design:  
The Building Blocks of a Good  
Experiment**

**Ann L. Oberg**  
Mayo Clinic



5:45 - 6:30 pm  
**Metabolite Profiling at the 'Omic'  
Scale: Untargeted Does not Mean  
Unplanned**

**Gary Patti**  
Washington University, St Louis

### SUNDAY CONFERENCE OPENING, 6:45 - 7:45 PM

Hall 5, level 1



**Welcome**  
**Vicki H. Wysocki**  
The Ohio State University  
ASMS Vice President for Programs



**The Human Gut Microbiome and  
Healthy Growth**

**Jeffrey L. Gordon**  
Washington University, St. Louis School  
of Medicine

### SUNDAY WELCOME RECEPTION, 7:45 - 9:00 PM

Poster/Exhibit Hall. Conference name badge is required.

## PLENARY SESSIONS

### MONDAY, 4:45 - 5:30 PM

#### AWARD LECTURE

Hall 5, level 1



**Award for a Distinguished  
Contribution in Mass Spectrometry**

**Brian T. Chait**  
The Rockefeller University

### TUESDAY, 4:45 - 5:30 PM

#### AWARD LECTURE

Hall 5, level 1



**Biemann Medal**

**Michael J. MacCoss**  
University of Washington

### THURSDAY, 4:45 - 5:30 PM

#### PLENARY LECTURE

Hall 5, level 1



**The Evolution of Modern  
Neurosurgery: A History of Trial and  
Error, Success and Failure**

**G. Michael Lemole, Jr.**  
The University of Arizona College of  
Medicine

### DON'T MISS

#### • ASMS MEETING, WEDNESDAY, 4:45 - 5:30 PM

Ballroom 222/224, level 2

Enjoy a beverage while you applaud awards, hear about new initiatives, and more!

#### • CLOSING EVENT, THURSDAY, 6:30 - 9:00 PM City Museum

*Let's celebrate!* Your adventure begins with a maze of turrets and open "tunnels" that lead to views of fantastic structures and sculptures. Try your skills of balance and courage, through caves and impossible slides. End with a surprise "artist" and St. Louis buffet. Buses will depart from the convention center, Washington Avenue entrance. Ticket is required, \$30.





**ORAL SESSIONS** are 8:30 - 10:30 am and 2:30 - 4:30 pm Monday through Thursday.

**Level 1**

- Session A (MOA, TOA, WOA, ThOA)..... Hall 5
- Session B (MOB, TOB, WOB, ThOB) ..... Room 130/132
- Session C (MOC, TOC, WOC, ThOC) ..... Room 123/124
- Session D (MOD, TOD, WOD, ThOD) ..... Room 120/127
- Session E (MOE, TOE, WOE, ThOE) ..... Theater
- Session F (MOF, TOF, WOF, ThOF)..... Room 106

**Level 2**

- Session G (MOG, TOG, WOG, ThOG) . Ballroom 222/224
- Session H (MOH, TOH, WOH, ThOH) .. Ballroom 220/221

**ORAL PRESENTATIONS** are projected from ASMS computers running Microsoft Office 2010. Speakers are required to use the ASMS computers for their presentations.

**SPEAKERS** must load presentations at least one day prior to their talks. The speaker room is 116, level 1 between Hall 4 and 5. The room is open with a technician according to this schedule:

- Sunday:** 10:00 am - 8:00 pm
- Monday through Thursday:** 7:30 am - 2:00 pm

**POSTERS AND EXHIBIT BOOTHS** are in the Poster/Exhibit Hall. The Hall is open:

- Sunday Reception .....7:45 pm - 9:00 pm
- Monday - Wednesday .....7:30 am - 8:00 pm
- Thursday .....7:30 am - 3:00 pm

**POSTER SET-UP** is 7:30 am on the day scheduled. Refer to the poster numbers in this final program for board assignments. A counter for poster supplies is near the main entrance to the Hall.

**POSTER SESSIONS** are 10:30 am - 2:30 pm, Monday through Thursday.

**POSTER AUTHORS** must be present at posters on scheduled days at these times.

- 10:30 am - 1:00 pm ..... Odd-numbered posters
- 12:00 - 2:30 pm ..... Even-numbered posters

Presenters who must leave a poster unattended should post a return time. Presenters should wear "Poster Presenter" badges which are available at the poster supply counter.

Posters should not be removed before 7:30 pm on Monday, Tuesday and Wednesday. Thursday posters should be removed at 2:30 pm.

**LUNCH CONCESSIONS** in the Poster/Exhibit hall offer a variety of options to dine and network while taking a break from posters. Concessions are open 11:00 am - 2:00 pm, Monday through Thursday.

**EXHIBITORS** must staff exhibit booths as follows:

- Sunday Reception .....7:45 pm - 9:00 pm
- Monday - Thursday ..... 10:30 am - 2:30 pm

**WORKSHOPS** are 5:45 - 7:00 pm on Monday, Tuesday, and Wednesday. Light refreshments are provided in the pre-function areas on level 1 and outside ballroom on level 2.

**DINNER BREAK, 7:00 - 8:00 PM** is time for a breath of fresh air before the opening of hospitality suites at 8:00 pm.

**SPECIAL PROGRAM FOR UNDERGRADUATE STUDENTS**

- **Sunday, 7:30 - 9:00 pm, Poster competition,** Poster/Exhibit Hall
- **Monday, 11:30 am - 1:00 pm, Meet the Experts.** lunch tables reserved for undergraduate students in the Poster/Exhibit Hall, Free vouchers for lunch will be provided at the tables. Arrive promptly at 11:30 am to obtain your voucher.
- **Wednesday, 5:45 - 7:00 pm, Workshop: Getting the Most out of Undergraduate Research in Mass Spectrometry,** Room 230

**FREE WiFi ACCESS** is provided in the Poster/Exhibit Hall. Computers are provided at stations throughout the convention center.

**CONFERENCE PROCEEDINGS** will be published online. Visit [www.asms.org](http://www.asms.org) after July 6 to view or download the Proceedings. Submission to the Proceedings does not constitute publication and does not jeopardize the rights of authors to publish contents of their submissions. **Speaker web casting slides will be printed to PDF and used for speakers who fail to submit.**

**WEB CASTING** includes tutorial lectures, plenary lectures, and oral sessions. Web casting will be available to conference attendees for three months after the conference. ASMS does not retain rights to material included in web castings. To access the presentations, go to [www.asms.org](http://www.asms.org) and log in. After login, go to annual conference page and select "web casting." Web casting button is visible only to conference registrants.

**CORPORATE HOSPITALITY SUITES** may be open 8:00 - 11:00 pm, Monday through Wednesday. Suites are located in the **Renaissance Grand Hotel.**

**CAREER CENTER** is located near the Washington Avenue entrance. The Career Center is open to all conference attendees. Applicants and employers must enter resumes and employment opportunities online. There are computers in the center for searching the database of candidates and positions. Interview rooms must be reserved one day in advance.

- Sunday .....7:45 - 9:00 pm
- Monday – Wednesday .....7:30 am - 5:00 pm
- Thursday .....7:30 am - 2:30 pm

**GUEST REGISTRATION** (\$10) includes designated name badge and entrance to the Sunday evening reception. The badge does not gain entrance to oral sessions or the Poster/Exhibit Hall.

**CONCIERGE DESK** in the conference registration area offers information on transportation, attractions and restaurants.



## GENERAL INFORMATION

**CORPORATE BREAKFAST SEMINARS** are hosted by some Corporate Members. Breakfast seminars are located on level 2 of the convention center and seats must be reserved in advance. **Please reserve at company exhibit booths.**

MONDAY	
Company	Convention Center Room
Advanced Chemistry Development (ACD)	Room 242
Agilent Technologies	Room 276
Bruker Daltonics	Room 263/264
LECO	Room 241
SCIEX	Room 265/266
SCIEX	Room 275
Shimadzu	Room 274
Thermo Scientific (in Renaissance Hotel)	Landmark 4-7
Waters	Room 230
Waters	Room 231
TUESDAY	
Company	Convention Center Room
Agilent Technologies	Room 276
Biotage	Room 231
Bruker Daltonics	Room 263/264
EMD Millipore	Room 240
GL Sciences	Room 265/266
LECO	Room 241
New Objective	Room 242
Phenomenex	Room 230
Promega	Room 261/262
Prosolia	Room 232
SCIEX	Room 275
SCIEX (in Renaissance Hotel)	Majestic D
Shimadzu	Room 274
Thermo Scientific (in Renaissance Hotel)	Landmark 4-7
Waters	Room 260/267
WEDNESDAY	
Company	Convention Center Room
Agilent Technologies	Room 276
Bruker Daltonics	Room 263/264
LECO	Room 241
New Objective	Room 242
Promega	Room 261/262
SCIEX	Room 265/266
SCIEX	Room 275
Shimadzu	Room 274
Thermo Scientific (in Renaissance Hotel)	Landmark 4-7
Waters	Room 230
Waters	Room 231
THURSDAY	
Company	Convention Center Room
Shimadzu	Room 274
Thermo Scientific	Room 276

**CORPORATE MEDIA EVENTS** are for members of the press and financial institutions. All will be held in the Renaissance Grand Hotel.

Company	Monday	Renaissance Hotel Location
Shimadzu	8:00-9:00 am	Majestic F-H
Bruker	9:30-10:30 am	Majestic A-C
SCIEX	11:00 -12:00 pm	Majestic D
Agilent Technologies	1:30-2:30 pm	Landmark 1-3
Thermo Scientific	3:00-4:00 pm	Landmark 4-7
Waters Corporation	4:30-5:30 pm	Majestic E

### CONFERENCE REGULATIONS

- Name badge is required for all conference sessions, including the Poster/Exhibit Hall and the employment center.
- No smoking is permitted in the convention center.
- Cell phones must be turned off in oral sessions.
- No photography or recording is allowed in oral sessions or in the poster/exhibit Hall.
- Material presented or displayed at the ASMS Conference, including but not limited to orals, posters, workshops, exhibit booths and hospitality suites, is the intellectual property of the presenter and may not be recorded, photographed, quoted, disseminated or transmitted by summary in any form without the express written authority of the author of the material presented. Such materials that are published in print or online must contain appropriate credits for all quotations and photographs.
- The placement of advertising in the meeting area is prohibited. There are poster boards and tables in the Poster/Exhibit Hall for approved announcements. No signs on easels are permitted.
- Hardware, accessories or any items for sale may be displayed only in corporate exhibit booths and hospitality suites.
- No organized activities (even off-site) other than those approved by ASMS are allowed during the conference week (5:00 pm on Sunday through 6:00 pm on Thursday).
- Corporate or institutional logos on slides or posters may appear only one time in the presentation.

# HOTELS



## CONFERENCE HOTELS

Hotel	Telephone
*Crowne Plaza Downtown	314-621-8200
*Drury Plaza at the Arch	314-231-3003
Drury Inn & Suites Conv Ctr	314-231-8100
Embassy Suites	314-269-5900
*Hampton Inn Gateway Arch	314-621-7900
*Hilton Ballpark	314-421-1776
*Hilton Downtown	314-436-0002

Hotel	Telephone
Holiday Inn (formerly Ramada Plaza)	314-421-5974
*Hyatt Regency Magnolia	314 655 1234
*Union Station St. Louis - A Doubletree by Hilton Hotel	314-621-5262
Renaissance Grand	314-621-9600

*\*Shuttle service to/from the convention center and hospitality suites will be provided from these hotels.*



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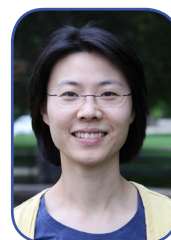
to these members who were elected to the ASMS Board

*Vice President for Arrangements*



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Advion, Quintiles and Cornell University  
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<i>Forensics &amp; Homeland Security</i>	Glen Jackson Guido Verbeck
<i>FTMS</i>	Nathan Kaiser Don Smith
<i>Fundamentals</i>	Alessandra Ferzoco Jos Oomens
<i>H/D Exchange, Covalent Labeling &amp; Cross Linking</i>	Joshua Sharp David Weis
<i>Imaging MS</i>	Vilmos Kertesz Zoltan Takats
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<i>Ion Trap MS</i>	Daniel E. Austin
<i>Lipids &amp; Lipodomics</i>	Stephen Blanksby
<i>LC/MS Related Topics</i>	Michael Bereman Helene Cardasis
<i>Metabolomics</i>	Andrew Patterson Sunia Trauger
<i>Metal Ion Coordination Chemistry</i>	Benjamin Bythell Alex Shvartsburg
<i>Pharmaceuticals</i>	Christine Gu Shawna Hengel
<i>Photoionization MS</i>	Jack Syage Ralf Zimmerman
<i>Polymeric Materials</i>	Stephen Rumbelow Gyorgy Vas
<i>Regulated Bioanalysis</i>	Jian Wang
<i>Undergraduate Research in MS</i>	Elaine Marzluff J.C. Poutsma
<i>Young Mass Spectrometrists</i>	Olga Friese Kristin Wildsmith

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<i>Sanibel Conference</i>	JC Poutsma, Chair Erin Baker Patrick Griffin Fanyu Meng

**ARCHIVIST**

Michael Grayson

## AWARD FOR A DISTINGUISHED CONTRIBUTION IN MASS SPECTROMETRY

2015 RECIPIENT: BRIAN T. CHAIT

AWARD LECTURE: 4:45 PM, MONDAY, HALL 5, LEVEL 1



**Dr. Brian T. Chait** is awarded the 2015 ASMS Award for a Distinguished Contribution in Mass Spectrometry for the recognition and demonstration of the link between protein structure and conformation and electrospray ionization mass spectra. His discovery that a protein's solution phase conformation impacts its electrospray ionization mass spectrometry (ESI-MS) charge state distribution (CSD) blasted away the barriers isolating mass spectrometry from its ability to probe higher order macromolecular structures and fostered a continuing deluge of applications of MS to noncovalent assemblies, hydrogen/deuterium exchange, probes of gas-phase protein structure, and ultimately "native mass spectrometry."

Today, interpreting ESI-MS and MS/MS data for proteins examined from native solutions often begins from NMR or crystal structures, based on assumptions that the gas-phase structure will not be too distant. But 24 years ago there was no expectation that relationships from higher order solution structure could be retained in the gas phase and any such assumption would have been foolhardy. The Chait laboratory opened the world to this possibility, first by demonstrating that electrosprayed cytochrome *c* molecules assumed about twice as much charge when sprayed from pH 2.6 than from pH 5.2 H<sub>2</sub>O (*J. Am. Chem. Soc.* 112, 9012 (1990)), by probing conformational changes in proteins via hydrogen/deuterium exchange (*Rapid Commun. Mass Spectrom.* 5, 214 (1991)), and by monitoring solution-phase thermal denaturation processes by ESI-MS (*Anal. Chem.* 65, 1, (1993)).

Dr. Chait's achievement must be viewed from the perspective of mass spectrometry in 1990 when few of us were capable of spraying 100% aqueous solutions, or did we see a need for it. For some of us an organic sheath solvent (or make-up flow) reduced surface tension enough to complete our analyses; others simply added methanol directly. However, Chowdhury and Chait (*Anal. Chem.* 63, 1660 (1991)) demonstrated that electropolished needles could electrospray water at voltages sufficiently below those inducing dielectric breakdown. That ability to electrospray 100% H<sub>2</sub>O was key to observing the charge state distribution differences associated with natively folded proteins. Equally important was Dr. Chait's ability to rationalize and prove that the source of the observed CSD difference had to be solution-phase structure.

We know so little about electrospray ionization today; we knew even less 25 years ago, yet the ideas that Dr. Chait precisely articulated about the electrospray CSD/conformation relationship were a turning point for biological mass spectrometry.

Dr. Brian T. Chait is the Head of the Laboratory of Mass Spectrometry and Gaseous Ion Chemistry and a Camille and Henry Dreyfus Professor at The Rockefeller University, New York, NY.

## RON A. HITES AWARD OUTSTANDING RESEARCH PUBLICATION IN JASMS

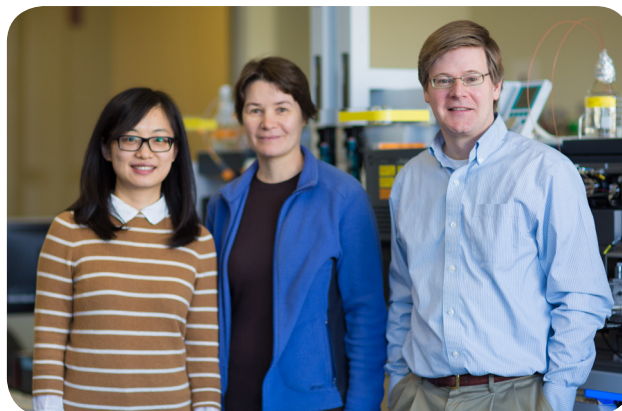
AWARD PRESENTATION: ASMS MEETING, 4:45 PM, WEDNESDAY, BALLROOM 222/224



The Ron Hites Award recognizes an outstanding publication of original research, based on a paper's innovative aspects, technical and presentation quality, likely stimulation of future research and impact on future applications. The award is named to honor Professor Ron Hites of Indiana University, who led the creation of JASMS in 1988 while president of ASMS. The award includes \$2,000 and a certificate for each author.

The 2015 award recognizes **John Klassen**, University of Alberta, and co-authors Lan Liu, Alyson Baergen, Klaus Michelsen, Elena N. Kitova, and Paul D. Schnier; for their paper Energetics of Intermolecular Hydrogen Bonds in a Hydrophobic Cavity: *JASMS*, 2014, 25, 742-750.

Left to right: Lan Liu, Elena Kitova, and John Klassen







## BIEMANN MEDAL

2015 RECIPIENT: MICHAEL J. MACCOSS

AWARD LECTURE: 4:45 PM, TUESDAY, HALL 5, LEVEL 1



**Dr. Michael J. MacCoss** has made a number of contributions of serious and long lasting impact to the field of proteomics. Chief among these is software development that has greatly facilitated proteomics. Dr. MacCoss' philosophy on making software freely available and continually supporting this software so that it enables others has greatly benefitted the proteomic sciences.

Bioinformatics tools developed by the MacCoss laboratory facilitate many different aspects of mass spectrometry data analysis. This includes tools for liquid chromatography mass spectrometry (LC-MS) feature finding, spectrum library searching, peak detection, post-processors for peptide database searching, and more. An important early contribution from his lab, the Percolator algorithm, improved peptide identifications from proteomic analyses through semi-supervised machine learning (Käll *et al.* "Semi-supervised learning for peptide identification from shotgun proteomics datasets," *Nature Methods*, 2007). Percolator became widely adopted partially because of its use of a liberal open source license that encouraged companies to build on Percolator and incorporate into commercial packages (e.g. Mascot and Proteome Discoverer). Another high-impact contribution from the MacCoss laboratory is the development and continued support of an integrated set of software

tools called Skyline (MacLean *et al.* "Skyline: an open source document editor for creating and analyzing targeted proteomics experiments" *Bioinformatics*, 2010; available from <http://skyline.maccosslab.org>). Critically, Skyline is a vendor-neutral toolset, thus enabling methods to be easily transferred and tested across labs, even those that utilize different instrument platforms. Dr. MacCoss has also substantially advanced the new area of data-independent MS analyses. His key contribution in this area has been to develop a multiplexed strategy to better isolate noise and improve signal detection and therefore sensitivity through observational coherence (Egertson *et al.*, *Nature Methods* 2013).

One of the most recent projects championed by Dr. MacCoss is a nonprofit to provide a cost effective mechanism for labs to backup, share, visualize, and analyze data on the cloud called The Chorus Project (<http://chorusproject.org>). They are working with developers in academic labs and companies to offer tools to our community that can process mass spectrometry data stored within Chorus. The hope is to provide a platform where all labs have access to the latest analysis tools and published data can be easily reanalyzed.

Dr. MacCoss is professor in the Department of Genome Sciences, University of Washington, Seattle.

## 2015 RESEARCH AWARDS

AWARD PRESENTATION: 4:45 PM, TUESDAY, HALL 5

The Research Awards are fully funded by Thermo Scientific and Waters Corporation in the amount of \$35,000 each.

Sponsored by  
THERMO SCIENTIFIC



**Michael Bereman**  
North Carolina State University

Sponsored by  
WATERS CORPORATION



**Alexander Ivanov**  
Northeastern University

## 2015 POSTDOCTORAL AWARDS

AWARD PRESENTATION: ASMS MEETING, 4:45 PM, WEDNESDAY, BALLROOM 222/224

Three awards in the amount of \$10,000 each are intended to promote the professional career development of postdoctoral fellows in the field of mass spectrometry. Activities funded by these awards include conference and workshop attendance, travel to other mass spectrometry laboratories, purchase of books and/or software. The awards are open to ASMS members who are postdoctoral fellows within three years of completing a Ph.D. or equivalent degree. Applicants must be currently appointed as a postdoctoral fellow in North America (e.g., in academia, industry, a government or national laboratory or at a research institute). Details and an application are posted to [asms.org](http://asms.org).



**Martin Paine**  
Georgia Institute of Technology



**Valentina Pirro**  
Purdue University



**Gloria Sheynkman**  
Harvard Medical School

## STUDENT AWARDS

AWARD PRESENTATION: ASMS MEETING, 4:45 PM, WEDNESDAY, BALLROOM 222/224

2015 inaugurates two student conference travel awards. There are seven awards of \$1,000 for graduate students and ten awards of \$500 for undergraduates. Applications and details for these awards are posted to [asms.org](http://asms.org). The deadline for submission is January 15.

## GRADUATE STUDENT AWARDS

**Benjamin Diner**  
Princeton University

**Albert Konijnenberg**  
University of Antwerp

**Xin Liu**  
University of Notre Dame

**Mandy Phelps**  
University of North Texas

**Nicholas Riley**  
University of Wisconsin-Madison

**Vincent Sica**  
University of North Carolina-Greensboro

**Chih-Chiang Tsou**  
University of Michigan

## UNDERGRADUATE STUDENT AWARDS

**Quintin Ferraris**  
Kean University

**Joshua Fischer**  
Wayne State University

**James Keating**  
University of Michigan

**James Matilla**  
James Madison University

**Danielle McDougall**  
University of Florida

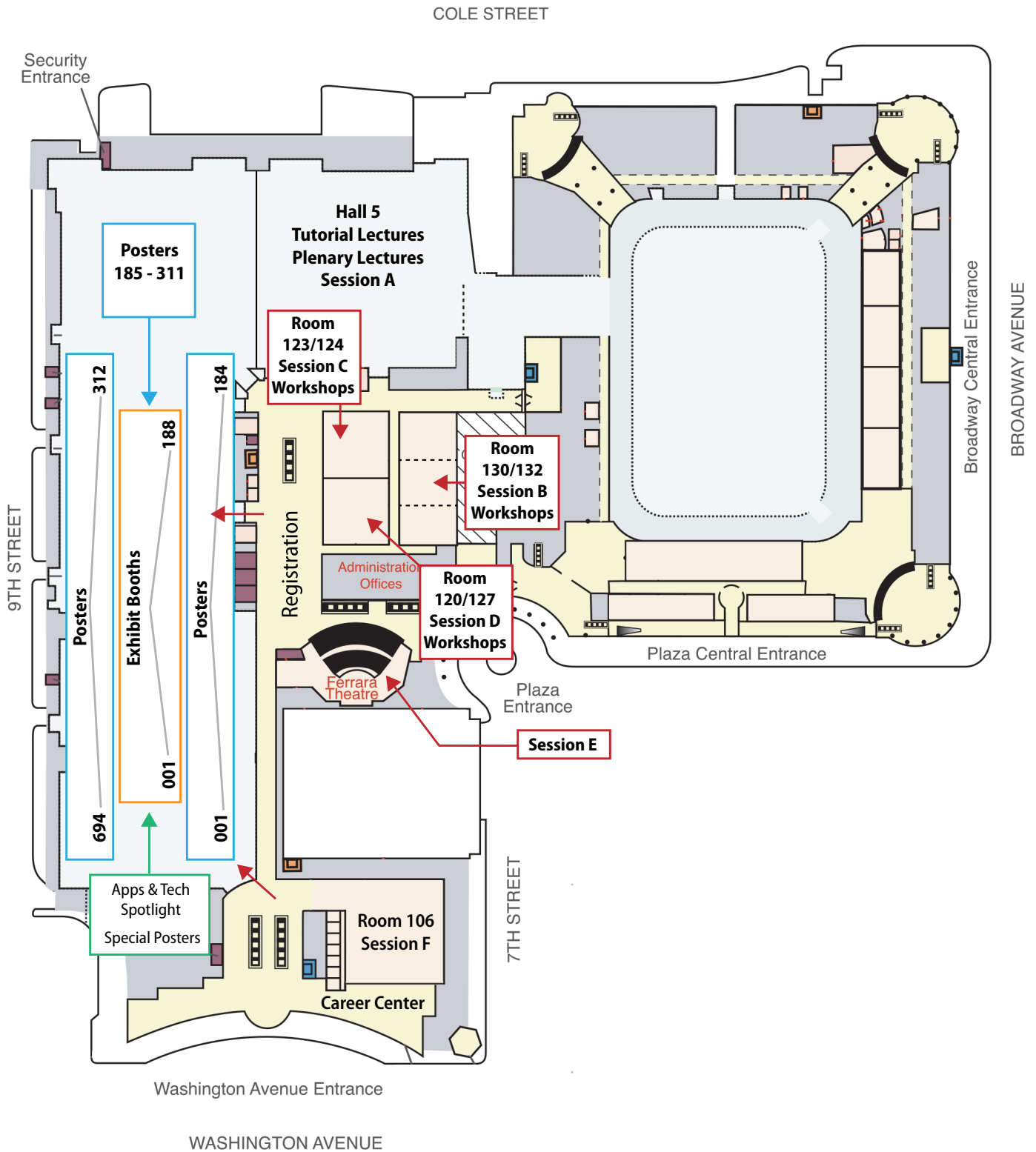
**Haley Miller**  
Bowdoin College

**Sydney Morris**  
George Washington University

**Alexandra Plaviak**  
Duquesne University

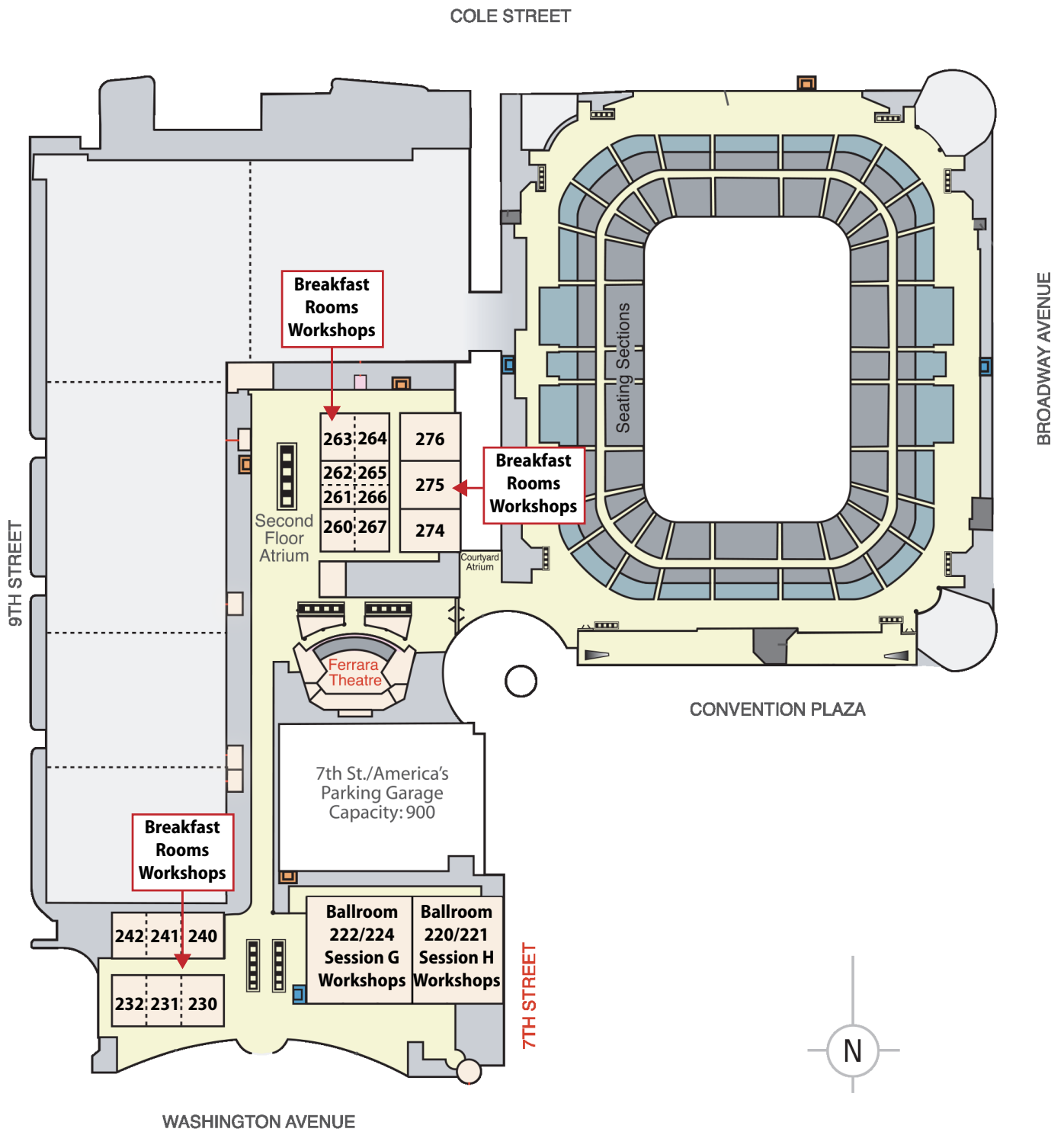
**Cheylene Tanimoto**  
Stanford University

**Nick van Huizen**  
Erasmus MC



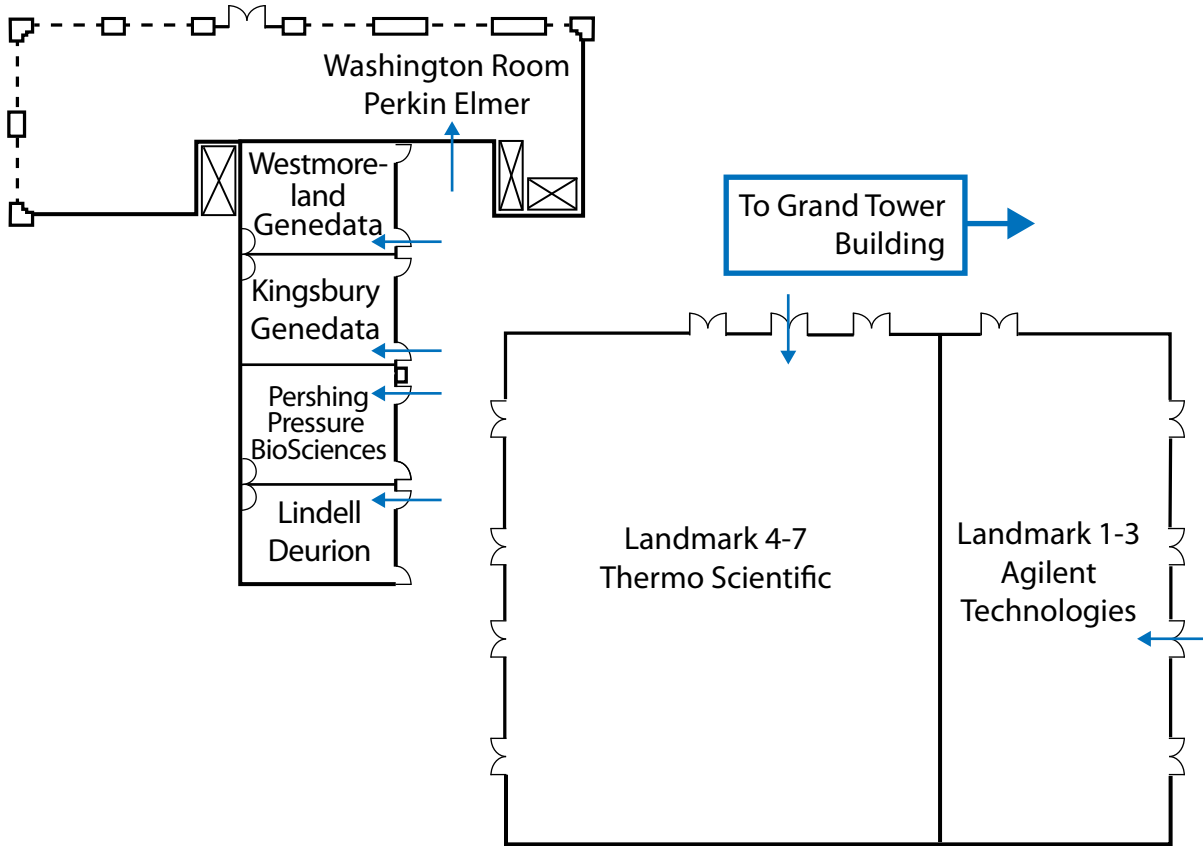


# AMERICA'S CENTER, LEVEL 2

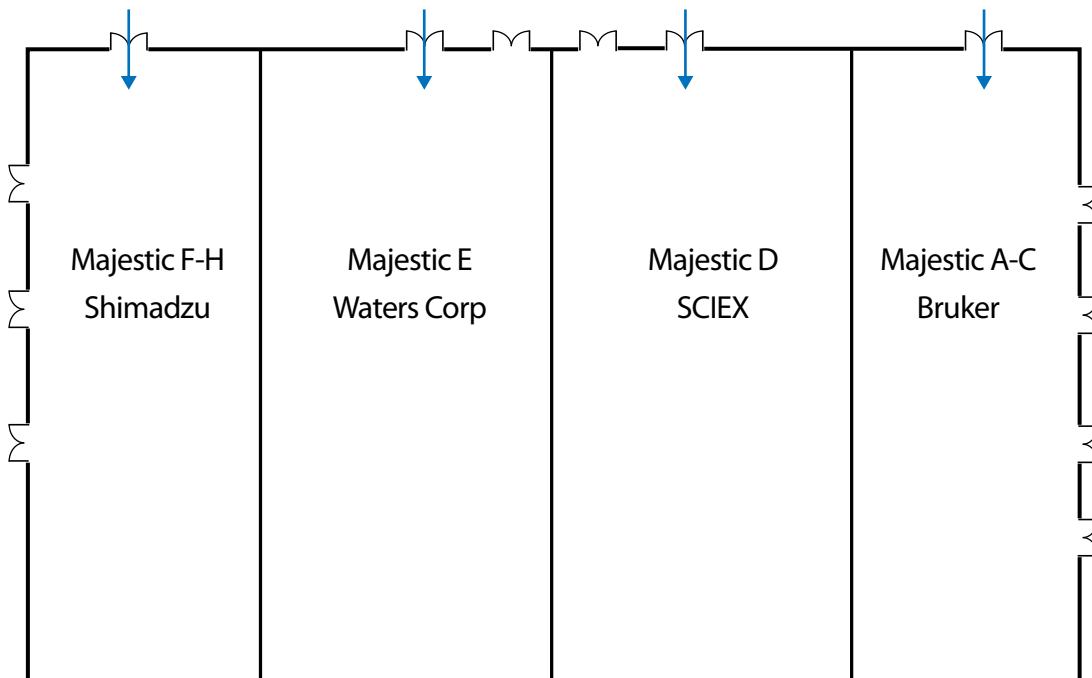




### Ballroom Complex – Lobby Level



### Ballroom Complex – Second Floor





## ASMS CORPORATE MEMBERS

COMPANY	POSTER / LIBRARY	BOOTH	SUITE IN RENAISSANCE HOTEL	BREAKFAST
ACS Publications	Library			
Advanced Chemistry Development (ACD/Labs)	Poster	83		Room 242, Monday (6/1)
Advanced Chromatography Technologies Ltd		52		
Advanced Energy		19		
Advion Inc.		171		
Agilent Technologies	Poster	141	Landmark 1-3	Room 276, Mon - Wed (6/1 - 6/3)
AIM Research Company		106		
American Pharmaceutical Review	Library			
Amsterdam Scientific Instruments		36		
Analytical Sales and Services, Inc.		22		
Anasys Instruments		32		
Antec	Poster	61		
Apricot Designs, Inc.		155		
Ardara Technologies LP	Poster	103		
Atlas Antibodies AB		107		
Avanti Polar Lipids, Inc.		79		
BaySpec, Inc.		97		
BIOCRATES Life Sciences AG		102		
Biognosys		132		
Bioinformatics Solutions Inc.	Poster	151		
BioPharma Services, Inc.		54		
Biotage		121		Room 231, Tuesday (6/2)
Biotech Support Group		73		
Bruker Daltonics		40	Majestic A-C	Room 263/264, Mon - Wed (6/1 - 6/3)
Busch Vacuum Pumps and Systems		48		
CAMAG Scientific, Inc.		145		
Cambridge Isotope Labs		179		
Canadian Life Science	Poster	162		
CAS		55		
Cayman Chemical Company		175		
Cell Signaling Technology		51		
Cerilliant	Poster	33		
Cerno Bioscience		178		
CovalX		81		
CSS Analytical Co. Inc.		11		
CTC Analytics AG		117		
Denator AB		146		
Detector Technology, Inc.		27		

## ASMS CORPORATE MEMBERS



COMPANY	POSTER / LIBRARY	BOOTH	SUITE IN RENAISSANCE HOTEL	BREAKFAST
Deurion			Lindell	
Dikma Technologies, Inc		68		
Drummond Scientific		105		
Edwards Vacuum		114		
Elforlight Ltd.		12		
EMD Millipore		84		Room 240, Tuesday (6/2)
EPREP		62		
ES Industries		136		
ESI Source Solutions		50		
ETP Electron Multipliers		44		
Excellims Corporation	Poster	59		
Exelis	Poster	87		
Expedeon		126		
Extrel		38		
FLIR Systems, Inc.	Poster	37		
Fluid Management Systems	Poster	10		
Fortis Technologies Ltd	Poster	177		
GAA Custom Engineering	Poster	3		
Genedata		119	Westmoreland/ Kingsbury	
Genetic Engineering & Biotechnology News	Library			
Genovis	Poster	90		
GenTech Scientific, Inc.		17		
GERSTEL, Inc.	Poster	94		
GL Sciences Inc.		39		Room 265/266, Tuesday (6/2)
Glygen Corp.		99		
Golden West Biologicals, Inc.		158		
Hamamatsu Corporation	Poster	148		
Hamilton Robotics		71		
Harvard Apparatus				
Hecate Software, Inc.		3		
Horizon Technology, Inc.		77		
HTX Technologies, LLC		78		
Hudson Surface Tech	Poster	35		
iChrom Solutions		9		
IDEX Health & Science	Poster	180		
iLab Solutions		6		
Imtakt USA		159		
Institute for Systems Biology		56		
INTAVIS Bioanalytical Instruments AG		95		
Integrated Engineering Software		74		



## ASMS CORPORATE MEMBERS

COMPANY	POSTER / LIBRARY	BOOTH	SUITE IN RENAISSANCE HOTEL	BREAKFAST
Integrated Proteomics Applications		89		
International Ceramic Engineering		29		
International Equipment Trading Ltd.		150		
ionBench		1		
Ionicon	Poster	163		
IONICS Mass Spectrometry		134		
IonSense, Inc.	Poster	110		
IsoSciences		7		
JEOL USA, Inc.		65		
JPT Peptide Technologies		69		
LEAP Technologies	Poster	30		
LECO Corporation	Poster	139		Room 241, Mon - Wed (6/1 - 6/3)
Linden CMS		131		
Mac-Mod Analytical		28		
Markes International	Poster	53		
MasCom Technologies		8		
MassTech Inc.		70		
Matrix Science		166		
Matsusada Precision Inc.		80		
McKinley Scientific		137		
MeCour Temperature Control		174		
Microliter Analytical Supplies (A WHEATON Company)		93		
Microsaic Systems		45		
Moeller Medical GmbH		176		
Molecular Discovery, Ltd		125		
Morpho Detection Inc.	Poster	133		
MS Bioworks		112		
MS Noise		170		
MS Vision		130		
MSParts		135		
mSPEC group		18		
MStm		156		
Nacalai USA, Inc.		104		
nanoLiter, LLC	Poster	57		
Nest Group, The	Poster			
New England Biolabs		66		
New England Peptide, Inc.		153		
New Objective, Inc.	Poster	138		Room 242, Tues - Wed (6/2 - 6/3)
NexTech Science Innovations, LLC		172		
NIST		25		
Novilytic		72		



## ASMS CORPORATE MEMBERS



COMPANY	POSTER / LIBRARY	BOOTH	SUITE IN RENAISSANCE HOTEL	BREAKFAST
Oerlikon Leybold Vacuum		109		
OmicScouts GmbH	Poster	88		
Omni International		124		
OPOTEK, Inc.		67		
Optimize Technologies, Inc.	Poster	144		
Owlstone, Inc.		165		
Pall Laboratory		43		
Parker Hannifin	Poster	91		
PEAK Scientific	Poster	143		
Perfinity Biosciences		157		
PerkinElmer		161	Washington (Mon, Tues only)	
Pfeiffer Vacuum	Poster	20		
Phenomenex		173		Room 230, Tuesday (6/2)
Phoenix Pharmaceuticals, Inc.		127		
Phoenix S&T, Inc.		101		
PHOTONIS	Poster	41		
Phytronix Technologies, Inc.		24		
PREMIER Biosoft		100		
Pressure BioSciences, Inc.		147	Pershing	
Promega Corporation		111		Room 261/262, Tues - Wed (6/2 - 6/3)
Prosolia, Inc.		64		Room 232, Tuesday (6/2)
Protea Biosciences, Inc.		123		
Protein Metrics Inc.		116		
Proteinaceous	Poster			
Proteome Software Inc.		31		
Proton Onsite		122		
Prozyme, Inc.		49		
PTM Biolabs, Inc.		129		
Pursuits Instrument Limited		115		
Resolution Systems, Inc.		108		
Restek Corporation		152		
RMI Laboratories		164		
Sage Science, Inc.		16		
Samin Science Co., Ltd		15		
Science/AAAS	Library			
Scientific Instrument Services	Poster	2		
Scientific Systems, Inc.		34		
SCIEX		21	Majestic D	Room 275, Mon - Wed (6/1 - 6/3); Rm 265/266, Mon & Wed (6/1, 6/3); Renaissance Hotel Majestic D, Tues (6/2)
Shimadzu Scientific Instruments, Inc.	Poster	120	Majestic F-H	Room 274, Mon - Thurs (6/1 - 6/4)



## ASMS CORPORATE MEMBERS

COMPANY	POSTER / LIBRARY	BOOTH	SUITE IN RENAISSANCE HOTEL	BREAKFAST
Shrader Software Solutions	Poster	75		
Sierra Analytics		128		
Silantes GmbH		5		
Sound Analytics		14		
Spark Holland	Poster	167		
SpectralWorks Limited	Poster	118		
Spectroscopy		142		
Spellman High Voltage		58		
Springer Science + Business Media		149		
SunChrom GmbH		98		
Supelco	Poster	92		
Tandem Labs		169		
Tecan		46		
The Analytical Scientist	Library			
Thermo Scientific		140	Landmark 4-7	Renaissance Hotel Landmark 4-7, Mon-Wed (6/1-6/3); Room 276, Thursday (6/4)
Tofwerk AG		23		
Tomtec		13		
Tosoh Bioscience		168		
Trajan Scientific and Medical		26		
TSI Inc.		96		
United Science Corp.		154		
Veritomyx		113		
VICI Valco Instruments		85		
VRS		42		
WarpLCMS		86		
Waters Corporation	Poster	160	Majestic E	Room 260/267, Tues (6/2); Room 230, Mon & Wed (6/1, 6/3); Room 231 Mon & Wed (6/1, 6/3)
Wiley	Library			
Worldwide Clinical Trials		47		
XPC Corporation		60		
YMC America, Inc.	Poster	82		
Zef Scientific Inc.		63		
Zhejiang Haochuang Biotech Co., Ltd		76		

## PROGRAM ACKNOWLEDGEMENTS



**Vicki H. Wysocki**  
The Ohio State University  
*Vice President for Programs*

### STUDENT ASSISTANTS

Graduate students and postdoctoral fellows assist with many aspects of the conference, including registration, oral and poster sessions, and the employment center. The students each receive a stipend to help with their conference travel expenses.

### PROGRAM COMMITTEE

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Abraham Badu-Tawiah Nicolas Brunelli Hao Chen Charles (Guilong) Cheng Allison Dill	Ashok Dongre Michael Freitas Sophie Harvey Chengsi (Michelle) Huang Yue Ju	Young-Jin Lee John McLean Royston Quintyn Nilini Ranbaduge Kevin Schey	Arpad Somogyi Yang Song Akiko Tanimoto Will Thompson Yu Xia Liwen Zhang
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### SESSION CHAIRS

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Abraham Badu-Tawiah Douglas F. Barofsky Dana B. Barr Mark P. Barrow Ian Blair Carolyn J. Cassady Steve Castellino Robert Chalkley Julia Chamot-Rooke Timothy Croley Darren Dumlao Kent Ervin Kenyon Evans-Nguyen Lee Ferguson David Ford Valérie Gabelica	Hongying Gao Kevin Giles Kari Green Leslie M. Hicks Christopher L. Holliman Xiaoping Hronowski Lan Huang Matthew Hurt A. Daniel Jones Kaveh Jorabchi Richard King Oliver Kohlbacher Lars Konermann Arthur Laganowsky Carlito Lebrilla Alexander Leitner	Jihyeon Lim Brendan MacLean Jody C. May Mark McComb Erkinjon Nazarov Alexey Nesvizhskii Peter Nemes Eugene Nikolaev William Noble Zheng Ouyang Akhilesh Pandey Melvin Park Natasha Penner Jim Prell Jun Qu Ragu Ramanathan	Susan Richardson Birgit Schilling Oliver Serang Michal Sharon Christine Snozek Frank Sobott Erik Soderblom Liangliang Sun Zoltan Takats Gary Van Berkel Derek Wilson H. Ewa Witkowska Keyang Xu Zhibo Yang Kangling Zhang Wendy Zhong Mingshe Zhu
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### WORKSHOP ORGANIZERS

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Sue Abbatiello Daniel Austin Erin Baker Alain Balland Kevin Bateman Michael S. Bereman Stephen Blanksby Andrey Bondarenko Jennifer Brodbelt Matthew Bush Benjamin Bythell Chris Colangelo Timothy Croley Eric Deutsch Brent Dixon Dawn Dufield	Christer Ejsing Marc Engel Alessandra Ferzoco Olga Friese Chris Gill Tim Griffin Christine Gu Walter Hammack Shawna Hengel Jason Hogan Damian Houde Nate Kaiser Vilmos Kertesz Sangtae Kim Skip Kingston	Bernhard Kuster Michael MacCoss Anthony Macherone Elaine Marzluff Luis Mendoza Mehdi Moini Jos Oomens Ron Orlando Andrew Patterson Brett Phinney Brian Rappold Stephen Rumbelow Nalini Sadagopan Joshua Sharp David Shteynberg	Alexandre Shvartsburg Vincent Sica Don Smith Jack Syage David Tabb Zoltan Takats Sunia Trauger Stephen Valentine Mustafa Varoglu Gyorgy Vas Guido F. Verbeck Jian Wang David Weis Kristin Wildsmith Matthias Wilhelm Nathan Yates
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## PROGRAM OVERVIEW

### SATURDAY

9:00 AM - 4:30 PM	<b>SHORT COURSES</b>
2:00 - 5:00 PM	<b>REGISTRATION</b>

### SUNDAY

9:00 AM - 4:30 PM	<b>SHORT COURSES</b>
10:00 AM - 8:00 PM	<b>REGISTRATION</b>
4:00 - 4:45 PM	<b>ATTENTION! FIRST-TIME GRADUATE STUDENTS AND UNDERGRADUATE STUDENTS</b> Plan your Strategy: What to See and Do at ASMS
5:00 - 6:30 PM	<p><b>TUTORIAL LECTURES</b>, Hall 5, level 1</p> <div style="display: flex; align-items: flex-start; margin-top: 10px;"> <div style="flex: 1;">  </div> <div style="flex: 2; padding-left: 10px;"> <p><b>5:00 - 5:45 pm</b> Statistical Experimental Design: The Building Blocks of a Good Experiment</p> <p><b>Ann L. Oberg</b> Mayo Clinic</p> </div> </div> <div style="display: flex; align-items: flex-start; margin-top: 10px;"> <div style="flex: 1;">  </div> <div style="flex: 2; padding-left: 10px;"> <p><b>5:45 - 6:30 pm</b> Metabolite Profiling at the 'Omic' Scale: Untargeted Does not Mean Unplanned</p> <p><b>Gary Patti</b> Washington University, St Louis</p> </div> </div>
6:45 - 7:45 PM	<p><b>CONFERENCE OPENING</b>, Hall 5, level 1</p> <p><b>Vicki Wysocki</b>, <i>ASMS Vice President for Programs</i></p> <div style="display: flex; align-items: flex-start; margin-top: 10px;"> <div style="flex: 1;">  </div> <div style="flex: 2; padding-left: 10px;"> <p><b>7:00 - 7:45 pm</b> The Human Gut Microbiome and Healthy Growth</p> <p><b>Jeffrey L. Gordon</b> Washington University St. Louis School of Medicine</p> </div> </div>
7:45 - 9:00 PM	<b>RECEPTION IN THE POSTER/EXHIBIT HALL</b> Undergraduate Student Poster Competition

## PROGRAM OVERVIEW



### MONDAY

<b>7:30 AM - 5:00 PM</b>	<b>REGISTRATION</b>
<b>8:30 - 10:30 AM</b>	<b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>• MOA am: Instrumentation: New Developments in Ionization &amp; Sampling, Hall 5</li> <li>• MOB am: Informatics: Algorithmic and Statistical Advances, Room 130/132</li> <li>• MOC am: Protein Complexes: Activation &amp; Dissociation, Room 123/124</li> <li>• MOD am: Glycopeptides and Glycoproteins, Room 120/127</li> <li>• MOE am: Metabolomics: New MS Technologies and Applications, Theater</li> <li>• MOF am: Quantitative Proteomics in Systems Biology/Cellular Pathway Analysis, Room 106</li> <li>• MOG am: Energy, Petroleum, &amp; Biofuels: Advances in MS Design &amp; Informatics, Ballroom 222/224</li> <li>• MOH am: Advances in Software and Hardware to Improve DMPK Workflows, Ballroom 220/221</li> </ul>
<b>10:30 AM - 2:30 PM</b>	<b>POSTER SESSION AND EXHIBITS</b> , Poster/Exhibit Hall, level 1 Monday posters 11:30 – 1:00 pm: <b>Undergraduate students</b> – look for reserved tables and free lunch vouchers to <i>Meet the Experts</i>
<b>2:30 - 4:30 PM</b>	<b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>• MOA pm: Ion Mobility, FAIMS &amp; DMS: New Developments &amp; Applications, Hall 5</li> <li>• MOB pm: Informatics: Metabolomics, Room 130/132</li> <li>• MOC pm: Top-Down Protein Analysis, Room 123/124</li> <li>• MOD pm: Plant-omics, Room 120/127</li> <li>• MOE pm: Clinical Diagnostics, Theater</li> <li>• MOF pm: PTMs: Advances in Isolation, Enrichment, Derivatization &amp; Separation, Room 106</li> <li>• MOG pm: Imaging: Biomedical Applications, Ballroom 222/224</li> <li>• MOH pm: Quantitative Analysis in Drug Discovery for Small Molecules, Ballroom 220/221</li> </ul>
<b>4:45 - 5:30 PM</b>	<b>AWARD LECTURE</b> , Hall 5, level 1 <b>Award for a Distinguished Contribution in Mass Spectrometry</b>  <b>Brian T. Chait</b> The Rockefeller University
<b>5:45 - 7:00 PM</b>	<b>WORKSHOPS</b> There are light refreshments in common areas. <ol style="list-style-type: none"> <li>01. Has Photoionization Reached its Potential? Focus on APPI, Room 130</li> <li>02. Enabling Proteomics Informatics on the Amazon Cloud, Room 131</li> <li>03. Advanced MS and Separation Approaches for Biofuels and Petroleum, Room 132</li> <li>04. The Galaxy Framework for MS-based Informatics, Room 123/124</li> <li>05. Defining Resolution in Imaging MS - A Quest for Solid Ground, Room 120/127</li> <li>06. Ion Traps: New Experiments and Old Tricks, Room 260/267</li> <li>07. Metal Cationization of Biomolecules and its Analytical Applications, Room 274</li> <li>08. Methods and Tools for Intra- and Inter-Experiment LC MS Performance Tracking, Room 275</li> <li>09. Challenges and progress towards the Site-Specific Characterization of Glycoprotein Heterogeneity, Room 230</li> <li>10. Mass Spectrometry Applications in Art, Cultural Heritage, and Natural History, Room 231</li> <li>11. More DMPK Knowledge from Less Sample: Leveraging Modern LC-MS Instruments for Small Sample Amounts, Room 232</li> <li>12. Metabolomics: Emerging Technologies for Continued Innovation, Ballroom 222/224</li> <li>13. Which Career Path is Right for Me? Ballroom 220/221</li> </ol>
<b>7:00 - 8:00 PM</b>	<b>DINNER BREAK</b>
<b>AFTER 8:00 PM</b>	<b>CORPORATE HOSPITALITY SUITES</b> , Renaissance Grand Hotel



## PROGRAM OVERVIEW

### TUESDAY

<b>7:30 AM - 5:00 PM</b>	<b>REGISTRATION</b>
<b>8:30 - 10:30 AM</b>	<b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>• TOA am: Instrumentation: Time-of-Flight and QTOF, Hall 5</li> <li>• TOB am: Informatics: Multi-omics Integration, Room 130/132</li> <li>• TOC am: Imaging: Instrumentation &amp; Method Development, Room 123/124</li> <li>• TOD am: Membrane Proteins, Room 120/127</li> <li>• TOE am: Lipidomics: New MS Technologies and Applications, Theater</li> <li>• TOF am: Phosphoproteomics in Disease, Room 106</li> <li>• TOG am: Emerging Environmental Contaminants, Ballroom 222/224</li> <li>• TOH am: LC-MS Approaches to Combine Translational PK/PD Biomarkers with Small Molecule ADME Workflows, Ballroom 220/221</li> </ul>
<b>10:30 AM - 2:30 PM</b>	<b>POSTER SESSION AND EXHIBITS</b> , Poster/Exhibit Hall Tuesday posters
<b>2:30 - 4:30 PM</b>	<b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>• TOA pm: New Developments in High Resolution and Mass Accuracy, Hall 5</li> <li>• TOB pm: Data Independent Acquisition: Innovative Methods and Applications, Room 130/132</li> <li>• TOC pm: Ion Spectroscopy, Room 123/124</li> <li>• TOD pm: Proteomics: Infectious Disease, Room 120/127</li> <li>• TOE pm: Lipids and Profiling, Theater</li> <li>• TOF pm: Protein-Protein and Protein-Ligand Interactions, Room 106</li> <li>• TOG pm: Environmental MS: Instrumental Challenges and Solutions, Ballroom 222/224</li> <li>• TOH pm: Imaging: Pharmaceuticals and Metabolites, Ballroom 220/221</li> </ul>
<b>4:45 - 5:30 PM</b>	<b>AWARD LECTURE</b> , Hall 5, level 1  <div style="display: flex; align-items: center;">  <div> <p><b>Biemann Medal</b></p> <p><b>Michael J. MacCoss</b> University of Washington</p> </div> </div>
<b>5:45 - 7:00 PM</b>	<b>WORKSHOPS</b> There are light refreshments in common areas <ol style="list-style-type: none"> <li>01. Laboratory Developed Test Guidance and Mass Spectrometric Diagnostics: Impact and Expectations, Room 130</li> <li>02. Current Trends, Gaps, and Needs in Workflows for Targeted Protein Quantitation by LC/MS, Room 131</li> <li>03. ProteomicsDB, Room 132</li> <li>04. FTMS: MS/MS at High Resolution, Room 123/124</li> <li>05. Identifying Tandem Mass Spectra of Lipids and Carbohydrates, Room 120/127</li> <li>06. MS Analysis of Antibody-Drug Conjugates, Room 260/267</li> <li>07. Measuring the Exposome: Strategies and Preliminary Results, Room 274</li> <li>08. Advancements and Discussion of Mass Spectrometry Technology and Challenges within the Polymer and Material Fields, Room 275</li> <li>09. The ABCs of Being a Great Reviewer for Scientific Journals, Room 230</li> <li>10. How to Network without Really Trying, Room 231</li> <li>11. Room 232</li> <li>12. Invalidating your Cores Data: Examples on How to Check your Data and Report Results and Communicate Invalid or Bad Results to your Customers, Room 222/224</li> <li>13. How Can Ion Mobility Spectrometry Separations Help your Research? Room 220/221</li> </ol>
<b>7:00 - 8:00 PM</b>	<b>DINNER BREAK</b>
<b>AFTER 8:00 PM</b>	<b>CORPORATE HOSPITALITY SUITES</b> , Renaissance Grand Hotel

## PROGRAM OVERVIEW



### WEDNESDAY

<b>7:30 AM - 5:00 PM</b>	<b>REGISTRATION</b>
<b>8:30 - 10:30 AM</b>	<b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>• WOA am: Ambient and Atmospheric Pressure Generation of Multiply-Charged Ionic Species, Hall 5</li> <li>• WOB am: Informatics: PRM &amp; DIA, Room 130/132</li> <li>• WOC am: Ion Mobility: Structures, Room 123/124</li> <li>• WOD am: Carbohydrates, Room 120/127</li> <li>• WOE am: FT, Ion Traps, and Hybrid Instruments, Theater</li> <li>• WOF am: Mass Spectrometry in Structural Biology, Room 106</li> <li>• WOG am: Epigenetic Modifications and Mechanisms, Ballroom 222/224</li> <li>• WOH am: Application of Stable Isotope Labeling in MS Analysis of Small Molecules and Proteins, Ballroom 220/221</li> </ul>
<b>10:30 AM - 2:30 PM</b>	<b>POSTER SESSION AND EXHIBITS</b> , Poster/Exhibit Hall Wednesday posters
<b>2:30 - 4:30 PM</b>	<b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>• WOA pm: Ambient Ionization: Instrumentation &amp; Applications, Hall 5</li> <li>• WOB pm: Informatics: Protein Identification and Quantification, Room 130/132</li> <li>• WOC pm: Reactions, Dynamics &amp; Theory of Gas Phase Ions, Room 123/124</li> <li>• WOD pm: Nucleic Acids, Room 120/127</li> <li>• WOE pm: Food Chemistry and Safety, Theater</li> <li>• WOF pm: H/D Exchange: Technologies and Applications, Room 106</li> <li>• WOG pm: Energy, Petroleum, &amp; Biofuels :Sample Preparation &amp; MS Interface Design, Ballroom 222/224</li> <li>• WOH pm: Antibodies and Anti-body Drug Conjugates, Ballroom 220/221</li> </ul>
<b>4:45 - 5:30 PM</b>	<b>ASMS MEETING</b> , Ballroom 222/224, level 2 Awards, board reports, wine, beer, soft drinks - and more!
<b>5:45 - 7:00 PM</b>	<b>WORKSHOPS</b> There are light refreshments in common areas. <ol style="list-style-type: none"> <li>01. The Role of High Resolution Mass Spectrometry in the Regulatory Environment, Room 130</li> <li>02. Emerging Contaminants for Emerging Scientists, Room 131</li> <li>03. Mass Spectrometry Instrumentation at the Forefront of Technology as Miscible Tools for Forensic and Security Evidence, Room 132</li> <li>04. Gas-Phase Ion Chemistry: Thermodynamics, Kinetics, Structures and Spectroscopy, Room 123/124</li> <li>05. Emerging Technologies Advancing Mass Spectrometry Research: 3D Printing, Room 120/127</li> <li>06. CHORUS - A Community Solution for the Storage Visualization, Sharing, and Analysis of Mass Spectrometry Data on the Cloud, Room 260/267</li> <li>07. The Big Fat Questions: The Future for Lipidomics in Cell Biology and Clinical Diagnostics? Room 274</li> <li>08. Characterization of Protein Therapeutics by Mass Spectrometry, Room 275</li> <li>09. Getting the Most out of Undergraduate Research in Mass Spectrometry, Room 230</li> <li>10. Working with Federal Agencies to Obtain Research Support : Mock NIH Study Section and Q&amp;A with Agency Staff, Room 231</li> <li>11. Room 232</li> <li>12. Ligand Binding Assays (LBA) and LC-MS/MS Integrated Antibody-Drug Conjugate (ADC) Bioanalysis -Immuno-capture LC-MS/MS Hybrid Assays: Challenges, Solutions, and Complementarity with LBA, Ballroom 222/224</li> <li>13. Hydrogen-Deuterium Exchange, Covalent Labeling and Crosslinking, Ballroom 220/221</li> </ol>
<b>7:00 - 8:00 PM</b>	<b>DINNER BREAK</b>
<b>AFTER 8:00 PM</b>	<b>CORPORATE HOSPITALITY SUITES</b> , Renaissance Grand Hotel



## PROGRAM OVERVIEW

### THURSDAY

<b>7:30 AM - 5:00 PM</b>	<b>REGISTRATION</b>
<b>8:30 - 10:30 AM</b>	<b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>• ThOA am: Mini/Portable/Fieldable MS, Hall 5</li> <li>• ThOB am: Informatics: Peptide Identification and Quantification, Room 130/132</li> <li>• ThOC am: New and Developing Ion Activation Methods, Room 123/124</li> <li>• ThOD am: Nano-Scale &amp; Microfluidic Separations &amp; MS, Room 120/127</li> <li>• ThOE am: Structure/Reactivity and Energetics of Gas-Phase Ions and Complexes, Theater</li> <li>• ThOF am: MS in Protein Footprinting: Michael Gross 75th Birthday, Room 106</li> <li>• ThOG am: Targeted Quantification of Proteins &amp; Post-Translational Modifications, Ballroom 222/224</li> <li>• ThOH am: Ion Mobility: Small Molecules, Pharmaceuticals, and DMPK, Ballroom 220/221</li> </ul>
<b>10:30 AM - 2:30 PM</b>	<b>POSTER SESSION AND EXHIBITS</b> , Poster/Exhibit Hall Thursday posters
<b>2:30 - 4:30 PM</b>	<b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>• ThOA pm: MS in Surgery, Hall 5</li> <li>• ThOB pm: Mult-PTMs: Comprehensive Analysis, Room 130/132</li> <li>• ThOC pm: Peptide Fragmentation and Peptidomics, Room 123/124</li> <li>• ThOD pm: Forensic Applications, Room 120/127</li> <li>• ThOE pm: Synthetic Polymers, Theater</li> <li>• ThOF pm: Chemical Cross-linking and Covalent Labeling, Room 106</li> <li>• ThOG pm: Ecological and Human Health Environmental Chemistry and Toxicology, Ballroom 222/224</li> <li>• ThOH pm: Applying New LC/MS Techniques to Solve Challenging Drug Metabolism Problems, Ballroom 220/221</li> </ul>
<b>4:45 - 5:30 PM</b>	<b>PLENARY LECTURE</b> , Hall 5, level 1  <div style="display: flex; align-items: center;">  <div> <p>The Evolution of Modern Neurosurgery: A History of Trial and Error, Success and Failure</p> <p><b>G. Michael Lemole, Jr.</b> The University of Arizona College of Medicine</p> </div> </div>
<b>6:30 - 9:00 PM</b>	<b>CLOSING EVENT, City Museum.</b> Ticket required





There are light refreshments in common areas.

**MONDAY WORKSHOPS, 5:45 - 7:00 PM**

**01. Has Photoionization Reached its Potential?**

**Focus on APPI**

**Photoionization Interest Group**

**Ralf Zimmerman and Jack Syage presiding**

**Room 130**

This will be the third year for a Photoionization (PI) workshop. Previous ones were very successful with strong turnout and varied and vigorous discussions. There are two flavors of photoionization currently being practiced today: (1) atmospheric pressure photoionization (APPI) is a commercial technology and practiced mostly on LC/MS instrumentation though there are vibrant growing new applications in direct ambient analysis, GC/MS and direct vapor (or vaporized) sample analysis. (2) Vacuum photoionization more commonly referred to as single-photon ionization (SPI) involves VUV light sources including lasers that ionize sample inside the vacuum chamber and is more of a research tool for studying spectroscopic properties of molecules, but also finding powerful applications in air monitoring particularly pollutant monitoring such as vehicle or flue exhaust.

In this third year we will focus on the topic of whether PI has reached its potential. This is an important topic because there are strong opinions that it is not used as much as its benefits warrant due to the entrenched use of common commercial ionization sources such as ESI and APCI. One can say that PI is late to the game. On the other hand PI and APPI are finding unique uses in high volume applications, most specifically explosives detection in security environments for its unique benefits that are not provided by competing ionization methods.

We have gotten some feedback discouraging us from trying to include both APPI and SPI topics because they are practiced by very different groups of users. So Ralf and I have decided to emphasize one or the other on alternate years. Not totally exclusive, but a strong emphasis and this year the emphasis will be on APPI.

**02. Enabling Proteomics Informatics on the Amazon Cloud**

**Eric Deutsch, Luis Mendoza, David Shteynberg presiding**

**Room 131**

The workshop will begin with a basic overview of the Trans-Proteomic Pipeline (TPP) and its newest features including new compute cloud concepts and services, primarily those offered by Amazon Web Services (AWS). We will describe the amztp platform, which facilitates the usage of AWS in the context of database searching using open-source engines as well as validation and analysis via the TPP; we will also conduct a live demo of the software. During the evening, we will conduct an open discussion on what other software tools and pipelines the community feels should be integrated into the amztp infrastructure (e.g. RNA-Seq analysis, SWATH data processing), and how to best provide an API and framework for others to incorporate their own tools that they wish to launch on the cloud.

**03. Advanced MS and Separation Approaches for Biofuels and Petroleum Energy, Petroleum & Biofuels Interest Group**

**Patrick Hatcher presiding**

**Room 132**

**04. The Galaxy Framework for MS-based Informatics**

**Tim Griffin presiding**

**Room 123/124**

The Galaxy framework for informatic workflow management has emerged as a useful tool for informatics and analysis of biological MS data. Originally focused on genomic informatics, Galaxy enables deployment of disparate software programs into a user-friendly environment, where software tools can be integrated into useful workflows. Once developed, the complete workflows and software tools can be easily shared with other Galaxy users. Given these advantages, Galaxy has great potential to solve a variety of informatics challenges in biological MS.

This workshop will provide attendees a look at some emerging applications in biological MS that are challenging to researchers, and where Galaxy offers an informatics solution. Informal presentations will be given by experts on these applications, with a focus on providing useful details on how these software and workflows can be accessed and used immediately. Audience questions and discussion on usability and other issues will be fielded and facilitated. An informal panel discussion with the presenters will follow the presentations.

Presenters and expected topics will include:

- Gerben Menschaert (Ghent University) - "The Proteoformer Pipeline for RiboProfiling and MS-based Proteomics"
- Ira Cooke (La Trobe University)/Pratik Jagtap (University of Minnesota) - "Galaxy-based PeptideShaker tools and applications, with a focus on downstream applications"
- Shyamasree Saha (Queen Mary University of London) - "Targeted Proteomics tools in Galaxy"

Ample time will be offered for questions from attendees and discussion. Presenters will be available for an informal panel discussion in the final part of the workshop.

**05. Defining Resolution in Imaging MS:**

**A Quest for Solid Ground**

**Imaging MS Interest Group**

**Zoltan Takats and Vilmos Kertesz presiding**

**Room 120/127**

The central envisioned topic of the workshop will be "Spatial Resolution in Mass Spectrometry". Due to the recent introduction of a number of new technologies into Mass Spectrometric Imaging, a 'War of Numbers' broke out on the field, where individual research groups keep claiming better and better spatial resolution for their techniques or experimental setups. In order to establish a solid ground, the workshop makes an attempt to come up with a widely acceptable definition (and associated method of determining it!) for spatial resolution claimed in a scientific publication. Furthermore, we are planning to discuss the limitations on spatial resolution (and the associated relationship between sensitivity and resolution) in case of commercially available techniques. We are also planning to include a structural biology expert and end the workshop with a discussion on the concept of 'Necessary Resolution', i.e. the spatial resolution required to answer certain biological questions.

## MONDAY WORKSHOPS, 5:45 - 7:00 PM continued

Structure of the workshop is planned to follow these topics:

- Which resolution ? - the variety of definitions and protocols
- Discussion - coming to a commonly acceptable definition
- Resolution of commercially available techniques - trends and limitations
- The Necessary Resolution - what feature resolution and sensitivity is needed for answering biological questions?
- Discussion - Do MSI techniques meet these criteria?

**06. Ion Traps: New Experiments and Old Tricks**  
**Ion Trap MS Interest Group**  
**Dan Austin presiding**  
**Room 260/267**

Short talks and group discussion will focus on two topics:

1. exciting new experiments
2. tutorial/perspective talks about challenging aspects of trap design and operation.

**07. Metal Cationization of Biomolecules and its Analytical Applications**  
**Metal Ion Coordination Chemistry Interest Group**  
**Benjamin Bythell and Alex Shvartsburg presiding**  
**Room 274**

Mass spectrometry has been revolutionized since the 1980-s by the invention of soft sources such as electrospray ionization (ESI) and matrix-assisted laser desorption ionization (MALDI) that enabled intact ionization of increasingly large macromolecules. While ionization via attachment or withdrawal of one or more protons has been typical, addition of other charged groups (such as metal cations) is equally possible. Metalated biomolecules differ substantially from their protonated analogs in terms of isotopic distribution and thus MS spectral pattern, conformation, and hence ion mobility separation properties, and/or dissociation chemistry and consequently the products in MS/MS, which may have important analytical benefits. In particular, electron-transfer dissociation and similar direct mechanisms may fragment biomolecules cationized by a multiply-charged metal in a different manner than their polyprotonated analogs of same total charge. This workshop will encourage the discussion and adoption of novel analytical strategies that leverage metal cationization as an alternative to protonation in biological mass spectrometry.

**08. Methods and Tools for Intra- and Inter-Experiment LC MS Performance Tracking**  
**LC/MS & Related Topics Interest Group**  
**Michael S. Bereman and Brent Dixon presiding**  
**Room 275**

The liquid chromatography mass spectrometry interest group aims to provide a collaborative atmosphere for research scientists, applications chemists, biologists and mass spectrometrists to share/discuss concepts for successful technology application. A major effort in the LC MS/MS community is harmonization and application of quality control metrics to provide confidence and reproducibility in published laboratory results. The chair and co-chair will provide an interactive workshop with insights from experience while engaging the audience. Performance tracking is a key component of transferable science which is strengthened through quality metrics. Confidence in results both within and across experiments lends itself to further application of discoveries to current and future work.

With active input from the audience, the chair and co-chair will discuss methods for monitoring LC MS/MS performance including: acquisition method type (targeted vs. DDA), metrics monitored (fundamental ID free vs. ID metrics), frequency of evaluation, and type of standard employed (simple vs. complex). In addition, an emphasis will be placed on available tools and software for tracking LC MS/MS performance in a longitudinal fashion.

**09. Challenges and Progress towards the Site-Specific Characterization of Glycoprotein Heterogeneity**  
**Ron Orlando presiding**  
**Room 230**

An early step typically employed in the characterization of glycoprotein glycans involves the liberation of the glycans from the peptide backbone. While this process facilitates the characterization of the glycans, information on the glycan distribution at each site is lost. This workshop focuses on approaches that are used to characterize intact glycoproteins/glycopeptides so that information on the attachment points of each glycan is obtained. The discussion will include: "top down" approaches and enzymatic digestion(s) followed by gas-phase or solution phase separations both condensed and gas phase separations. The use of targeted SRM approaches will also be presented and discussed, as these allow site-specific heterogeneity to be determined in complex mixtures. Methods that permit isomeric structural determination, such as MS<sup>n</sup>, will also be discussed.

**10. Mass Spectrometry Applications in Art, Cultural Heritage, and Natural History**  
**Mehdi Moini presiding**  
**Room 231**

The purpose of this workshop is to discuss the application of mass spectrometry (MS) to art and cultural heritage objects, as well as natural history specimens. This will be an interactive workshop in which various subjects relevant to the application of MS to art and natural history specimens will be discussed in a casual, dialog format. A preliminary list of topics include: 1) Analysis of proteinaceous and organic specimens such as silk and wool textiles, leather and animal guts objects, bone and tissues, ink, paper, paint, coatings, binders, and wood. 2) Analysis of the fundamental factors that cause degradation and aging of natural history and art objects; identification of their deterioration markers, using degradation markers as clocks for dating objects, and studying environmental factors that affect deterioration. 3) Application of MS to paleo-organic matter such as fossilomics, amino acid racemization, and ancient DNA. 4) Forensic archeology. 5) Determination of the authenticity of art objects.

**11. More DMPK Knowledge from Less Sample: Leveraging Modern LC-MS Instruments for Small Sample Amounts**  
**DMPK Interest Group**  
**Mustafa Varoglu and Kevin Bateman presiding**  
**Room 232**

Mass spectrometer performance has dramatically improved over the past several years, however sampling techniques for bioanalytical and drug metabolism studies have remained much the same. This DMPK-IG workshop will explore combining mass spectrometer improvements with microsampling of plasma, tissues and miniaturized assays to create better workflows to increase the quality of the DMPK data, and advance drug discovery and development projects. Topics to be explored by panel members and the workshop participants include microsampling blood for


**MONDAY WORKSHOPS, 5:45 - 7:00 PM** continued

plasma or dried blood spot analysis, the translational advantages of serial microsampling vs. traditional sampling methods and the ability to miniaturize assays. In addition, the opportunities for obtaining early tissue distribution data from low amounts of tissue either by homogenization or microdialysis in discovery vs. waiting for comprehensive imaging via MS-imaging or QWBA techniques will be examined. This workshop will explore the opportunities and barriers of leveraging the full abilities of our modern mass spectrometers to take advantage of limited sample amounts.

**12. Metabolomics: Emerging Technologies for Continued Innovation**  
**Metabolomics Interest Group**  
**Sunia Trauger and Andrew Patterson presiding**  
**Ballroom 222/224**

The workshop will begin with brief presentations to stimulate discussion among the workshop participants. Emerging tools to facilitate metabolomics research and new technologies will be discussed. The moderators will highlight 2-3 recent developments in the field and survey the audience for their opinions. A panel of

invited scientists with expertise in field will be available to answer questions posed by the moderators and attendees. The workshop will close with a discussion where attendees can ask questions of the panelists. Some of the topics addressed will be: (i) new software tools for post-processing of untargeted metabolomics data, (ii) innovative experimental designs (iii) shotgun approaches with ion mobility, and (iv) metabolite identification by *in silico* fragmentation.

**13. Which Career Path is Right for Me?**  
**Young Mass Spectrometrists Interest Group**  
**Olga Friese and Dian Su presiding**  
**Ballroom 220/221**

The workshop features a panel discussion on professional development. Topics will be focused on career planning and management, fundamental training, industrial internship, job search tools and interview strategies. The panel, consisting of representatives from government, industrial and academic organizations, will share their knowledge and practices on career prospects.

There are light refreshments in common areas.

**TUESDAY WORKSHOPS, 5:45 - 7:00 PM**

**01. Laboratory Developed Test Guidance and Mass Spectrometric Diagnostics: Impact and Expectations**  
**Clinical Chemistry Interest Group**  
**Brain Rappold presiding**  
**Room 130**

In July 2014, the Food and Drug Administration released draft guidance on the use of laboratory developed tests (LDT's). With few exceptions, the use of mass spectrometry testing in patient care is performed by LDT's. The guidance requirements will impact all aspects of mass spectrometric testing in the clinic, from therapeutic drug monitoring to companion diagnostics. Additionally, the proposed guidance will affect the evolution of new biomarkers and new testing, particularly that of multi-index analyte tests. Representatives from manufacturing, industry, regulatory bodies and advocacy groups will deliver brief presentations on their considerations of the proposed directives, followed by an open forum in which the expectations for the industry to deliver on the submission of analytical platforms and assays to the agency will be discussed.

**02. Current Trends, Gaps, and Needs in Workflows for Targeted Protein Quantitation by LC/MS**  
**Nalini Sadagopan, Sue Abbatiello, and Dawn Dufield presiding**  
**Room 131**

With increase in focus on biologic/biotherapeutic drugs by the pharmaceutical industry and also an increase in need for biomarkers (efficacy and safety) the deployment of LC-MS based techniques is on the rise primarily due to the speed in method development, and specificity of the technique. Scientists are finding new ways of doing sample prep to increase sensitivity/specificity, address reproducibility issues associated with enzymatic digestion and mass spectrometric methods to address specificity. The forum will provide a platform to share common themes, issues on these fronts and perhaps to surface newer needs in software, mass spec design, and automation.

We conducted this workshop at ASMS 2014 in Baltimore for the first time and was very successful. We sent out a survey with the participants prior to ASMS and the summary of the survey results were presented. We had about 150 attendees. Panel discussion with industry experts and thought leaders with the audience engagement was valuable. There was interest in continuing this workshop for 2015.

**03. ProteomicsDB**  
**Bernhard Kuster and Mathias Wilhelm presiding**  
**Room 132**

There is a growing landscape of various databases and repositories for MS and proteomics. In this workshop, we would like to present recent and future developments ProteomicsDB, a free, professionally developed solution to store and analyze mass spectrometry-based proteomics data. ProteomicsDB has a strong focus on functionality and secondary use of proteomics and mass spectrometry data. Following up on a successful workshop at ASMS 2014, we would like to encourage the involvement from the ASMS community, demonstrate typical use-cases for the web interface and API and describe our short and long-term plans.

**04. FTMS: MS/MS at High Resolution**  
**FTMS Interest Group**  
**Nathan Kaiser and Don Smith presiding**  
**Room 123/124**

The workshop will focus on the practical aspects of tandem MS coupled to high resolution FTMS instruments. FTMS enables tandem MS experiments that are only capable on high resolution instruments. Applications that highlight these unique advantages will be discussed, such as top-down mass spectrometry by electron based methods (ETD/ECD), photo dissociation (UVPD), and collisional based methods (CID/CAD). The workshop will be open for discussion on applications, instrumentation, method development, and data analysis for high resolution tandem MS.

TUESDAY WORKSHOPS, 5:45 - 7:00 PM *continued*

**05. Identifying Tandem Mass Spectra of Lipids and Carbohydrates**  
**Bioinformatics Interest Group**  
**Sangtae Kim and David Tabb presiding**  
**Room 120/127**

In shotgun proteomics, the identification of tandem mass spectra is taken as a given, and database search algorithms have occupied center stage for two decades. Tandem mass spectra from lipids and carbohydrates, on the other hand, have enjoyed considerably less bioinformatics support. In this panel, the Bioinformatics Interest Group features an introduction to these classes of data from two researchers who have recently published algorithms to automate identification. Dr. Haixu Tang will discuss his efforts to recognize the structures of glycans and glycopeptides. Tomas Cajka will discuss the creation of the LipidBlast spectral library as a tool for recognizing lipids from LC-MS/MS experiments in multiple instrument platforms.

**06. MS Analysis of Antibody-Drug Conjugates**  
**Pharmaceuticals Interest Group**  
**Shawna Hengel and Christine Gu presiding**  
**Room 260/267**

Due to the success and of the 2013 and 2014 pharmaceutical interest group workshops, and continued interest in MS analysis of antibody-drug conjugates (ADCs), we propose a similar workshop for 2015. After a short informal presentation, less than ten minutes, the majority of the workshop would include an audience driven discussion with the opportunity to ask questions to a panel of experts. The organizers will have backup questions prepared for the panel to start or prompt the discussion if needed. The short presentation will provide an update on current workflows for ADC MS analysis and discuss details of the large range of characterization required for ADCs from initial MAb assessment to bioanalytical assay development. To identify potential panelists, gauge the level of interest of the ASMS community, and tailor the discussion we will send out a survey of open ended questions in April.

**07. Measuring the Exposome: Strategies and Preliminary Results**  
**The Exposomic Interest Group**  
**Anthony Macherone and Skip Kingston presiding**  
**Room 274**

Genome-wide association studies (GWAS) rarely report relative risks greater than 1.2 for significant SNPs and estimates determined via mining of published data reveal overall genetic risks of about 5% for cancer and 12% for heart disease. These data suggest that the majority of causative factors for chronic human disease is not genetic but rather exposures or some combination of exposures and the genome (G). The exposome (E) is defined as the lifetime sum of these external and internal exposures. Accordingly, 80% - 90% of chronic human diseases is determined by E and GxE (including epigenetics).

The exposome encompasses the other "omes." For example, when one measures the transcriptome, proteome, or metabolome, they are measuring a slice of the exposome. Moreover, the exposome seeks the causative factors of disease to mitigate and prevent disease from occurring. The exposome is therefore a quantity of critical interest if we are to discover the non-genetic causative factors of chronic human diseases in a comprehensive manner. Mass spectrometric and other technologies such as spectroscopy and remote ("smart") sensors will characterize the exposome in large, prospective cohorts and provide reliable information on

exposure-risk relationships. The exposome paradigm will facilitate the translation of applied research into educational, behavioral and policy-based, risk mitigating interventions.

This workshop will review mass spectrometric based assays designed to measure the exposome both from a discovery and from a targeted perspective and present real data from case / control studies for discussion.

**08. Advancements and Discussion of Mass Spectrometry Technology and Challenges within the Polymer and Material Fields**  
**Polymer and Material MS Interest Group**  
**Stephen Rumbelow and Gyorgy Vas presiding**  
**Room 275**

This workshop will focus on updating the group on recent work and challenges faced in the various fields such as academic, government, and industry. The focus of this group is polymer and material analysis utilizing various mass spectrometric techniques for both characterization and quantitation of oligomeric species. This workshop will explore the various ways that polymers and materials are not only analyzed themselves but also how they interact with other materials such as patients, and different type of products such as packaging and medical devices.

**09. The ABCs of Being a Great Reviewer for Scientific Journals**  
**Jenny Brodbelt presiding**  
**Room 230**

The peer review process is a critical step in the evaluation of original scientific manuscripts. This workshop will cover the nuts-and-bolts of the publication workflow with an emphasis on the peer review process. A panel of Editors will provide an inside look at how manuscripts are handled after submission, how reviewers are selected, and the role of the both authors and reviewers in the process. Tips for being a top reviewer will be covered, as well as how to become involved as a new reviewer.

**10. How to Network without Really Trying: A Forum for Current (and Future) Mass Spectrometrists in Industry**  
**Lucinda Cohen presiding**  
**Room 231**

Building on last year's successful "How to Succeed in Pharma without Really Trying" this workshop is designed to bring together mass spectrometrists from all environments including, but not limited to, mass spectrometry vendors, chemical, pharmaceutical, forensic and academic scientists. Attendees will be divided into small groups for break-out discussions on topics such as career transitions, work-life balance and mentoring. Participants will have the opportunity to rotate through these small group sessions in a "speed dating" format to discuss as many topics of interest as possible and enhance networking. Each small group will have an experienced scientist and facilitator. All are welcome. Attendees should bring business cards for distribution if possible.



**TUESDAY WORKSHOPS, 5:45 - 7:00 PM** continued

**12. Invalidating your Cores Data: Examples on How to Check your Data and Report Results and Communicate Invalid or Bad Results to your Customers**  
**Analytical Laboratory Managers Interest Group**  
**Brett Phinney and Chris Colangelo presiding**  
**Ballroom 222/224**

One of Richard Feynman's more famous quotes involved integrity of scientific data: "If you're doing an experiment, you should report everything that you think might make it invalid -- not only what you think is right about it; other causes that could possibly explain your results; and things you thought of that you've eliminated by some other experiment, and how they worked -- to make sure the other fellow can tell they have been eliminated."

This workshop will present strategies, examples (both good and bad) and discussion on how to report data from analytical core facilities to customers and collaborators including potential problems and caveats that might make the data invalid. Often this challenging aspect is overlooked and under appreciated. Collaborators often have only a cursory understanding of what you did and communicating what may be wrong with the data you generated can be daunting.

- Examples presented during this workshop may include
- Examples on communicating potential problems with your data

- How to temper expectations of collaborators when they get excited over initial results
- How to report inconclusive or odd results
- Examples on when your data was wrong and how you fixed it (or did not fix it)
- Examples where initial results conflict with subsequent results, and how you handled it

**13. How Can Ion Mobility Spectrometry Separations Help Your Research?**  
**Ion Mobility Interest Group**  
**Stephen Valentine, Matthew Bush and Erin Baker presiding**  
**Ballroom 220/221**

Over the last 20 years, ion mobility spectrometry (IMS) separations have been incorporated in many different instrument technologies such as DMA, FAIMS, drift tube IMS, traveling wave IMS, TIMS, SLIM, etc. With all of these different variations, many people have found confusion as to when to apply each technology. This workshop will focus on explaining several of the currently available IMS technologies and delve into the present applications being performed by each such as standalone IMS measurements and MS coupled metabolomic analyses, proteomic studies, and ion/ion reactions.

There are light refreshments in common areas.

**WEDNESDAY WORKSHOPS, 5:45 - 7:00 PM**

**01. The Role of High Resolution Mass Spectrometry in the Regulatory Environment**  
**Flavor Fragrance and Foodstuff Interest Group**  
**Walter Hammack and Tim Croley presiding**  
**Room 130**

Last year the discussion centered around GC/MS, specifically high resolution options for GC/MS, which remains a staple of the food and food-related laboratories. This year, we propose to continue where we left off last year and focus on the role that high resolution mass spectrometry will play in the regulatory environment. The FDA has issued a guidance document for the use of high resolution data and a number of state and local labs are also beginning to look at HR data as a possible tool. In addition, a number of people are using the term, "non-targeted screening" and we would like to address this term, and, hopefully, come to a consensus on the use of this language. As in the past two years we intend to invite researchers from local, state, academic and government to share their experiences and then have a group discussion.

**02. Emerging Contaminants for Emerging Scientists**  
**Environmental Interest Group**  
**Chris Gill and Marc Engel presiding**  
**Room 131**

This workshop will consist of up to 5 brief presentations from undergraduates, graduates and first-time post-doc researchers from industry, government and academia. The workshop will provide a forum to discuss their work, goals and any problems (up to 5 slides maximum). The forum is aimed at providing positive mentoring and feedback from the working group for the new generation of environmental mass spectrometrists.

**03. Mass Spectrometry Instrumentation at the Forefront of Technology as Miscible Tools for Forensic and Security Evidence**  
**Forensics and Homeland Security Interest Group**  
**Guido Verbeck and Glen Jackson presiding**  
**Room 132**

Mass Spectrometry is arguably one of the most definitive techniques used to confirm the constituents of illicit drugs, energetic materials, urine, blood and other forensic evidence. It is because of the high sensitivity, high peak capacity, and low identification error that mass spectrometry has exploded into portable and imaging applications, as well as shotgun databasing of potential new illicit chemistries. The recent introduction of ambient ionization techniques—which differ somewhat from traditional GC/MS—has raised questions about the admissibility of different MS methods in courtroom battles. For example, are forensic and security applications of ambient ionization held to a different standard than GC/MS or LC/MS counterparts? When developing these instruments and applications, is there sufficient method validation conducted to provide sufficient confidence in analyses? In the proposed workshop, we offer a panel discussion of new mass spectrometric methods and technologies for forensics and security applications, and how we can satisfy the scientific and legal requirements in this important and rapidly developing area. We will also discuss the developments of mass spectrometric standards and recommendations in the various NIST-OSAC forensic science subcommittees.



## WORKSHOPS

WEDNESDAY WORKSHOPS, 5:45 - 7:00 PM continued

### **04. Gas-Phase Ion Chemistry: Thermodynamics, Kinetics, Structures and Spectroscopy Fundamentals Interest Group** **Jos Oomens and Alessandra Ferzoco presiding** **Room 123/124**

The Fundamentals Interest Group has a long tradition of organizing the Fundamentals of Ion Chemistry Workshop, which is well attended each year. We gladly extend this tradition at the upcoming ASMS conference.

As was commonly done at workshops in the recent past, we intend to invite several especially junior researchers to give a brief and informal presentation on their recent work (5 slides max). These short presentations should address unpublished work, work in progress and focus on aspects of the work such as unsolved questions, difficulties, mysteries, etc. The last slide should not so much contain conclusions, but rather open questions, which serve as introduction to a discussion on the subject. From previous experience, this usually leads to interesting, thoughtful and entertaining discussions, often providing novel insights to the presenter.

### **05. Emerging Technologies Advancing Mass Spectrometry Research: 3D Printing** **Vincent Sica and Vilmos Kertesz presiding** **Room 120/127**

This workshop series concerns the use of technologies that support advancements in the field of mass spectrometry. With 3D printers becoming more accurate, reliable, and affordable, they are quickly finding their way into laboratories. This year's discussion will focus on the implementation of 3D printing to support mass spectrometry research.

A couple of 5-minute presentations showcasing applications of this technology will be followed by the discussion of the following topics:

1. Choice of hardware (Cost, Precision, Ease of use)
2. Choice of software (Design & Slicing)
3. Choice of material (Chemical compatibility, Durability, etc.)
4. Micro or macro applications (Are your prints designed for your lab or the MS community?)
5. Tips and tricks (Software or hardware related)
6. What improvements to 3D printing are necessary to further impact MS (New filament types? Higher resolution? etc.)

These discussions aim to not only educate on how to improve their research through 3D printing, but also to spark ideas on what the future may bring to the growing technologies of both 3D printing and mass spectrometry.

### **06. CHORUS - A Community Solution for the Storage Visualization, Sharing, and Analysis of Mass Spectrometry Data on the Cloud** **Andrey Bondarenko, Michael MacCoss, Christine Wu, and Nathan Yates presiding** **Room 260/267**

The sharing, public dissemination, and analysis of mass spectrometry data has become a major challenge. We would like to present a community effort to provide a sustainable and professionally developed solution to the mass spectrometry field's needs. The application provides an intuitive graphical user interface specifically developed to organize and visualize mass spectrometry data. Data can be uploaded and kept private, shared with a group of collaborators, or made entirely public. Over the

last two years CHORUS has gained almost 1000 users and these users have placed >55,000 data files into the service. We are now in the process of releasing new tools that will enable the analysis of data stored within CHORUS and improving the interaction of our data with existing client and server tools.

We have received a lot of feedback from our users and we have used this feedback to alter our development efforts. We would like to discuss improvements made to CHORUS over the last year and what new analysis capabilities have and are being added. We will discuss our goals and get feedback from the community on our current and long-term priorities.

### **07. The Big Fat Questions: The Future for Lipidomics in Cell Biology and Clinical Diagnostics?** **Lipids and Lipidomics Interest Group** **Stephen Blanksby and Christer Ejsing presiding** **Room 274**

Innovation in mass spectrometry has fueled the rapid expansion of lipidomics research over the last decade. Increasingly powerful instrumentation and accompanying software tools are now available to wide range of researchers around the world. This workshop will reflect on some of the big research questions in cell biology, biotechnology and clinical medicine and ask whether current mass spectrometry-based lipidomics can underpin future breakthroughs in these disciplines. The discussion will be led by a panel of experts who will opine on current impediments to development in their respective fields. Panellists will challenge participants to consider how lipid mass spectrometry can breakthrough such roadblocks and drive innovation in biochemical understanding, clinical diagnosis or novel therapeutics. Conceptual discussion will then be facilitated on whether currently available lipid mass spectrometry approaches can provide these answers or whether new technology is required.

### **08. Characterization of Protein Therapeutics by Mass Spectrometry** **Biotherapeutics Interest Group** **Damian Houde, Alain Balland, and Jason Hogan presiding** **Room 275**

This workshop will be a forum to discuss the current technical challenges and solutions for the characterization of protein therapeutics by mass spectrometry. Mass spectrometry is now used for protein characterization from discovery through product development. The workshop will lead off with a short background overview of a few topics ranging from protein modifications, higher-order structure characterization, protein batch comparability and biosimilarity, or protein production lot release to initiate a discussion. Recent advancements in instrumentation and software for data analysis and reporting may also be discussed.

### **09. Getting the Most out of Undergraduate Research in Mass Spectrometry** **Undergraduate Research in MS Interest Group** **Elaine Marzluff presiding** **Room 230**

This panel discussion, aimed at undergraduate students and their mentors, will focus on helping undergraduate students leverage their undergraduate research in mass spectrometry into successful experiences in graduate school and industry.



WEDNESDAY WORKSHOPS, 5:45 - 7:00 PM continued

**10. Working with Federal Agencies to Obtain Research Support : Mock NIH Study Section and Q&A with Agency Staff**  
**Charles G. Edmonds and Douglas M. Sheeley presiding**  
**Room 231**

**12. Ligand Binding Assays (LBA) and LC-MS/MS Integrated Antibody-Drug Conjugate (ADC) Bioanalysis -Immuno-capture LC-MS/MS Hybrid Assays: Challenges, Solutions, and Complementarity with LBA Regulated Bioanalysis Interest Group**  
**Jian Wang presiding**  
**Ballroom 222/224**

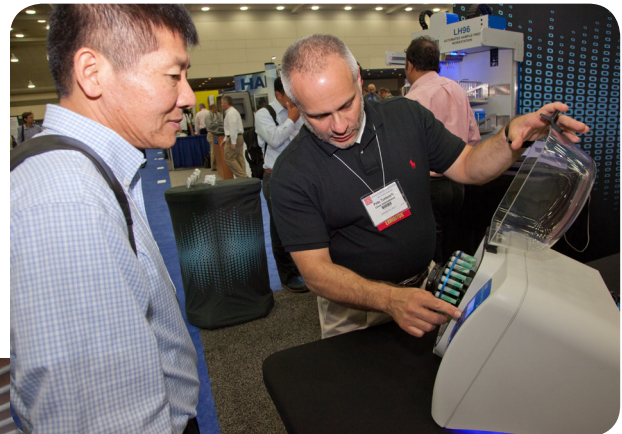
Antibody-drug conjugates (ADCs) consist of a cytotoxic drug covalently bound to an antibody (mAb) via a linker. The complex structure of ADCs presents unique bioanalytical challenges and requires novel strategies. Multiple analytes in the heterogeneous mixture may contribute to the efficacy and safety of ADCs. Four quantitative assays are considered essential, industry-wide, in ADC PK bioanalysis, (1) total-antibody, (2) conjugated-antibody, (3) conjugated-payload, and (4) unconjugated-payload. Immuno-capture LC-MS/MS hybrid assays are required for the analysis of conjugated-payload and are viable alternatives or complementary to ligand binding assays (LBA) for the analysis of total-antibody and conjugated-antibody.

Each hybrid assay involves three essential experimental steps: capture, enzymatic cleavage or digestion, and LC-MS/MS detection. After the initial immuno-capture of the ADC, the conjugated-payload assays proceed with the cleavage of the payload using Cathepsin B enzyme and LC-MS measurement of the released payload, while the conjugated-antibody and total-antibody assays measure the signature peptides generated by trypsin digestion of the mAb. Immuno-capture with either anti-id or anti-payload capture reagents could be conducted using magnetic beads or cartridges formats.

This workshop will focus on current hybrid assay strategies, applications, and their complementarity to ligand binding assays. Technical details of hybrid assay development and validation will be discussed. The capability of hybrid assays to appropriately quantify mixtures of analytes with different Drug to Analyte Ratio (DAR) will be addressed as well.

**13. Hydrogen-Deuterium Exchange, Covalent Labeling and Crosslinking Interest Group**  
**Joshua Sharp and David Weis presiding**  
**Ballroom 220/221**

The workshop will provide a forum for discussing the latest HDX, covalent labeling and crosslinking methods for protein analysis. The program will provide an opportunity to discuss MS-based methods, data analysis routines and applications with the attendees. The goal of the program will be to stimulate discussion and convey useful experimental detail you can take back to your lab.



## SUNDAY EVENING AND MONDAY MORNING ORAL SESSIONS

4:00 – 4:45 PM, SUNDAY  
Attention First-time Graduate Students and Undergrads  
Plan your Strategy: What to See and Do at ASMS  
Elaine Marzluff and JC Poutsma, presiding  
Ballroom 220/221

5:00 – 6:30 PM, SUNDAY  
TUTORIAL SESSION  
Vicki Wysocki (The Ohio State University) presiding  
Hall 5



5:00 – 5:45 pm  
Statistical Experimental Design:  
The Building Blocks of a Good Experiment

Ann L. Oberg  
Mayo Clinic



5:45 – 6:30 pm  
Metabolite Profiling at the 'Omic' Scale:  
Untargeted Does not Mean Unplanned

Gary Patti  
Washington University, St Louis

6:45 – 7:45 PM, SUNDAY  
Conference Opening  
Vicki Wysocki (The Ohio State University) presiding  
Hall 5

Welcome, Vicki Wysocki  
ASMS Vice President for Programs



The Human Gut Microbiome and Healthy  
Growth

Jeffrey L. Gordon  
Washington University, St. Louis School of  
Medicine

7:45 – 9:00 PM, SUNDAY  
WELCOME RECEPTION  
Poster/Exhibit Hall  
Conference name badge is required

### 8:30 – 10:30 AM, MONDAY MORNING INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION AND SAMPLING

Peter Nemes (George Washington University) presiding  
Hall 5

- MOA am 08:30 **Matrix Assisted Ionization: Enhancing Mass Spectrometry through Proper Sampling Conditions on Small Portable to High Performance Mass Spectrometers;** [Sarah Trimpin](#)<sup>1,2</sup>; Christian Reynolds<sup>1,2</sup>; Casey Foley<sup>1</sup>; Shubhashis Chakrabarty<sup>1,3</sup>; Daniel Woodall<sup>1</sup>; Jessica DeLeeuw<sup>1</sup>; Joshua Fischer<sup>1</sup>; Shameemah Thawoos<sup>1</sup>; Zachary Devereaux<sup>1</sup>; Bryan Harless<sup>1</sup>; Claudio Verani<sup>1</sup>; Mathew Allen<sup>1</sup>; Thomas Sanderson<sup>2</sup>; Karin Przyklenk<sup>2</sup>; Paul Stemmer<sup>4</sup>; <sup>1</sup>Department of Chemistry, Wayne State University, Detroit, MI; <sup>2</sup>Cardiovascular Research Institute, Wayne State Uni, Detroit, MI; <sup>3</sup>MSTM LLC, Wayne State University, Detroit, MI; <sup>4</sup>Institute of Environmental Health Science, WSU, Detroit, MI
- MOA am 08:50 **Infrared, Visible, and and Ultraviolet Laser Ablation for High Spatial Resolution Sampling Mass Spectrometry;** [Chinthaka A. Seneviratne](#); Suman Ghorai; Kermit K. Murray; Louisiana State University, Baton Rouge, LA
- MOA am 09:10 **Hybrid Optical Microscope/Laser Ablation Liquid Capture Mass Spectrometry System Providing Co-Registered Optical Bright Field, Fluorescence and Mass Spectral Images;** [Gary J. Van Berkel](#)<sup>1</sup>; John Cahill<sup>1</sup>; Vilmos Kertesz<sup>1</sup>; Thomas Covey<sup>2</sup>; Julian Burke<sup>3</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>ABSciex, Concord, Ontario, Canada; <sup>3</sup>Leica Microsystems Group, Cambridge, UK
- MOA am 09:30 **T-probe: a Novel Device to Implement Online in situ single Cell Analysis Using Mass Spectrometry;** [Renmeng Liu](#); Ning Pan; Zhibo Yang; University of Oklahoma, Norman, OK
- MOA am 09:50 **Fabrication of Silica Multi-nozzle Emitters for Multiple Electropray Ionization by Selective Etching of a Microstructured Fiber with Doped Regions;** [Yueqiao Fu](#)<sup>1</sup>; Timothy Hutama<sup>1</sup>; Graham Gibson<sup>1</sup>; Steeve Morency<sup>2</sup>; Jean-Francois Viens<sup>2</sup>; Younes Messaddeq<sup>2</sup>; Richard Oleschuk<sup>1</sup>; <sup>1</sup>Queen's University, Kingston, Canada; <sup>2</sup>COPL at Université Laval, Quebec City, Canada
- MOA am 10:10 **Square-Wave Facilitated Electroosmosis in a Theta Glass nESI Emitter: Improved Turbulent Mixing on the Milliseconds Timescale;** [Christine Fisher](#); Ryan T. Hilger; Feifei Zhao; Scott A. McLuckey; Purdue University, West Lafayette, IN

### 8:30 – 10:30 AM, MONDAY MORNING INFORMATICS: ALGORITHMIC AND STATISTICAL ADVANCES Oliver Serang (Thermo Fisher Scientific) presiding Room 130/132

- MOB am 08:30 **The Midpoint Mixed Model with a Missingness Mechanism: A Likelihood Based Framework for Relative Quantification of Mass Spectrometry Data;** [Jonathon O'Brien](#); Harsha P. Gunawardena; Bahjat Qaqish; University of North Carolina at Chapel Hill, Chapel Hill, NC
- MOB am 08:50 **Comparative Study of Automated Feature Selection and Classification Techniques For Detection of Histological Features by Mass Spectrometry Imaging;** [Nazanin Zounemat Kermani](#)<sup>1</sup>; Ottmar Golf<sup>2</sup>; Sabine Guenther<sup>1</sup>; Robert D. Goldin<sup>1</sup>; James Kinross<sup>1</sup>; Abigail V. M. Speller<sup>1</sup>; Kirill Veselkov<sup>1</sup>; Zoltan Takats<sup>1</sup>; <sup>1</sup>Imperial College London, London, UK; <sup>2</sup>Justus Liebig University, Giessen, Germany





- MOB am 09:10 **Multi-species Identification of Polymorphic Peptide Variants via Propagation in Spectral Networks;** Seungjin Na<sup>1</sup>; Sam Payne<sup>2</sup>; Nuno Bandeira<sup>1</sup>; <sup>1</sup>University of California, San Diego, La Jolla, CA; <sup>2</sup>Pacific Northwest National Lab, Richland, WA
- MOB am 09:30 **Clustering Spectra Based on Fragment Rarity;** Matthew The; Lukas Käll; Royal Institute of Technology - KTH, Stockholm, Sweden
- MOB am 09:50 **Improved Computational Demultiplexing for Data Independent Acquisition Data Acquired by MSX or with Overlapping Windows;** Jarrett Egerton<sup>1</sup>; Richard S. Johnson<sup>1</sup>; Yue Xuan<sup>2</sup>; Philip M Remes<sup>3</sup>; Brendan Maclean<sup>1</sup>; Gennifer Merrihew<sup>1</sup>; Olga Vitek<sup>4</sup>; Vlad Zabrouskov<sup>3</sup>; Markus Kellmann<sup>2</sup>; Michael J. Maccoss<sup>1</sup>; <sup>1</sup>Univ of Washington, Seattle, WA; <sup>2</sup>Thermo Fisher Scientific, Bremen, N/A; <sup>3</sup>Thermo Fisher Scientific, San Jose, CA; <sup>4</sup>Northeastern University, Boston, MA
- MOB am 10:10 **Improved Computational Analysis of Imaging Mass Spectrometry Data through Sparse Intensity Variation De-noising;** Yousef El Aalamat<sup>1,2</sup>; Nico Verbeeck<sup>1,2</sup>; Junhai Yang<sup>4</sup>; Bart De Moor<sup>1,2</sup>; Richard M. Caprioli<sup>4</sup>; Etienne Waelkens<sup>5,6</sup>; Raf Van De Plas<sup>3,4</sup>; <sup>1</sup>KU Leuven, ESAT-STADIUS, 3001 Leuven, Belgium; <sup>2</sup>Minds Medical IT, 3001 Leuven, Belgium; <sup>3</sup>Delft University of Technology, Delft, Netherlands; <sup>4</sup>Vanderbilt University, Nashville, TN; <sup>5</sup>KU Leuven, Dept. of Cellular and Molecular, 3000 Leuven, Belgium; <sup>6</sup>KU Leuven, SybioMa, 3000 Leuven, Belgium

**8:30 – 10:30 AM, MONDAY MORNING  
PROTEIN COMPLEXES: ACTIVATION & DISSOCIATION  
Michal Sharon (Weizmann Institute of Science) presiding  
Room 123/124**

- MOC am 08:30 **Assembly and Disassembly of Protein Complexes Involved in Complement Activation Monitored by Q-ToF and Orbitrap Analyzers with Extended Mass Ranges;** Guanbo Wang; Andrey Dyachenko; Albert J.R. Heck; Utrecht University, Utrecht, Netherlands
- MOC am 08:50 **On and Off: Probing Aβ Peptide Association with Aggregation Inhibiting Peptides and Small Molecules via Dissociation;** Ashley S. Phillips<sup>1</sup>; Harriet L. Cole<sup>2</sup>; Mark Taylor<sup>3</sup>; Isabel Riba-Garcia<sup>1</sup>; Cait E. MacPhee<sup>2</sup>; Richard D. Unwin<sup>1</sup>; Garth J. S. Cooper<sup>1</sup>; David Allsop<sup>3</sup>; Perdita E. Barran<sup>1</sup>; <sup>1</sup>University of Manchester, Manchester, UK; <sup>2</sup>University of Edinburgh, Edinburgh, UK; <sup>3</sup>University of Lancaster, Lancaster, UK
- MOC am 09:10 **Laser Activation of Soluble and Membrane Protein Assemblies for Structural Biology;** Victor A. Mikhailov; Idir Liko; Todd Mize; Carol Robinson; University of Oxford, Oxford, UK
- MOC am 09:30 **Surface Induced Dissociation Reveals Substructural Information Consistent With The Interfacial Analysis Of Protein Complexes;** Sophie R. Harvey; Royston S. Quintyn; Yang Song; Jing Yan; Aniruddha N. Sahasrabudde; Vicki H. Wysocki; The Ohio State University, Columbus, Ohio
- MOC am 09:50 **Determining Iron-Binding Motifs in Biological Macromolecular Assemblies with IR-Induced Native Electron Capture Dissociation;** Owen Skinner; Michael McAnally; Richard Van Duyn; Philip Compton; Neil L. Kelleher; Northwestern University, Evanston, IL

- MOC am 10:10 **Structural Interpretation of Gas-phase Protein Unfolding: New Applications in Structural Biology and Protein Engineering;** Joseph Eschweiler; Brandon Ruotolo; University of Michigan, Ann Arbor, MI

**8:30 – 10:30 AM, MONDAY MORNING  
GLYCOPEPTIDES AND GLYCOPROTEINS  
Xiaoping Hironowski (Biogen, Inc.) presiding  
Room 120/127**

- MOD am 08:30 **Isotope Targeted Glycoproteomics (IsoTaG): A Chemical Proteomics Platform for N- and O-Glycopeptide Discovery;** Christina Woo; Anthony Iavarone; Carolyn Bertozzi; UC Berkeley, Berkeley, California
- MOD am 08:50 **Integrated Bottom-Up and Middle-Down Glycoproteomics;** Kshitij Khatri; Joshua Klein; Yi Pu; Catherine E. Costello; Cheng Lin; Joseph Zaia; Boston University, Boston, MA
- MOD am 09:10 **O-GlcNAc Modification Site-Specific Characterization of ABL2 Produced from a ΔNagZ E. coli Co-Expression System by Tandem Mass Spectrometry;** Kelin Wang<sup>1</sup>; Octavia Y. Goodwin<sup>1</sup>; Fabrizio Donnarumma<sup>1</sup>; Behrooz Zekavat<sup>2</sup>; Touradj Solouki<sup>2</sup>; Megan A. Macnaughtan<sup>1</sup>; Kermit K. Murray<sup>1</sup>; <sup>1</sup>Louisiana State University, Baton Rouge, LA; <sup>2</sup>Baylor University, Waco, TX
- MOD am 09:30 **Glazer: An Integrated Software Platform for interpretation of N-glycopeptide MS/MS Data with Robust FDR Control, without ExD Dissociation;** John Froehlich; Peter Warren; Richard Lee; Children's Hospital Boston, Boston, MA
- MOD am 09:50 **Analysis of the Cell Surface N-Glycoproteome by Integrating Metabolic Labeling, Copper-free Click Chemistry and LC-MS/MS;** Johanna Smeekens; Weixuan Chen; Ronghu Wu; Georgia Institute of Technology, Atlanta, GA
- MOD am 10:10 **Top-down and Middle-Down CE-MS for Deep Characterization of Biopharmaceuticals with Glycan Heterogeneity: Identification of Interferon-β1 and Monoclonal Antibody Proteoforms;** David R. Bush<sup>1</sup>; Arseniy M. Belov<sup>1</sup>; Li Zhang<sup>2</sup>; Alexander R. Ivanov<sup>1</sup>; Barry L. Karger<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Biogen Idec, Inc., Cambridge, MA

**8:30 – 10:30 AM, MONDAY MORNING  
METABOLOMICS:  
NEW MS TECHNOLOGIES AND APPLICATIONS  
Ian Blair (University of Pennsylvania) presiding  
Theater**

- MOE am 08:30 TBD
- MOE am 08:50 **The Human Plasma REDOXOME: A Broad Compendium of Oxidative Stress Biomarkers;** Miriam Sindelar; Qiuying Chen; Darya Akimova; Ronald G Crystal; Steven S Gross; Weill Medical College of Cornell, New York, NY
- MOE am 09:10 **Metabolic Changes and Oxidative Stress Pathways in a Novel Patient Derived IDH1-R132H Mutant Oligodendroglioma Xenograft Assessed by Mass Spectrometry Imaging;** Guillaume Hochart<sup>1</sup>; Fred Fack<sup>2</sup>; Fabien Pamelard<sup>1</sup>; Jonathan Stauber<sup>1</sup>; Simone P. Niclou<sup>2</sup>; <sup>1</sup>ImaBiotech, MS Imaging Dept., Loos, France; <sup>2</sup>Luxembourg Institute of Health, Luxembourg, Luxembourg



## MONDAY MORNING ORAL SESSIONS

- MOE am 09:30 **Highly Reproducible and Robust LC-MS/MS Assay for Targeted Profiling of 180 Metabolites Using a Single HILIC Chromatography Method;** Danijel Djukovic<sup>1</sup>; Jiangjiang Zhu<sup>1</sup>; Haiwei Gu<sup>1</sup>; Farhan Himmati<sup>1</sup>; Daniel Raftery<sup>1,2</sup>; <sup>1</sup>University of Washington Medicine, Seattle, WA; <sup>2</sup>Fred Hutchinson Cancer Research Center, Seattle, WA
- MOE am 09:50 **Simultaneous Targeted Quantification and Untargeted Metabolomics of Meconium Steroid Content;** Nathaniel Snyder; Alexander Frey; Bo Young Park; *Drexel University, Philadelphia, PA*
- MOE am 10:10 **Effect of Controlled Diet on Biomarker Measurements in the Clinic;** Petia Shipkova; Serhiy Hnatyshyn; Michael Reilly; Yi Luo; Rose Christian; *Bristol Myers Squibb, Princeton, NJ*

### 8:30 – 10:30 AM, MONDAY MORNING

#### QUANTITATIVE PROTEOMICS IN SYSTEMS BIOLOGY/CELLULAR PATHWAY ANALYSIS

**Lan Huang (University of California, Irvine) presiding**  
Room 106

- MOF am 08:30 **PALM (Pulse Azidohomoalanine Labeling in Mammals) Analysis for Global Analysis of Newly-Synthesized Proteins in Animal Models of Disease;** John Yates<sup>1</sup>; Daniel Mclatchey<sup>1</sup>; Yuanhui Ma<sup>1</sup>; Reuben Shaw<sup>2</sup>; <sup>1</sup>The Scripps Research Institute, La Jolla, CA; <sup>2</sup>The Salk Institute, La Jolla, CA
- MOF am 08:50 **Refining the Human Proteome: Integrated Analysis of Human Tissues by RNAseq, Proteomics, Phosphoproteomics and Antibodies;** Hannes Hahne<sup>1</sup>; Dongxue Wang<sup>1</sup>; Björn Hallström<sup>2</sup>; Lihua Li<sup>1</sup>; Anna Asplund<sup>3</sup>; Mathias Wilhelm<sup>1</sup>; Harald Marx<sup>4</sup>; Frederik Ponten<sup>3</sup>; Mathias Uhlen<sup>2</sup>; Bernhard Kuster<sup>1</sup>; <sup>1</sup>Technical University Munich, Freising, Germany; <sup>2</sup>KTH Royal Institute of Technology, Stockholm, Sweden; <sup>3</sup>Uppsala University, Uppsala, Sweden; <sup>4</sup>University Wisconsin-Madison, Madison, WI
- MOF am 09:10 **An ORFeome-based, Mass Spectrometry-driven Human Protein Interaction Network;** Edward L. Huttlin<sup>1</sup>; Lily Ting<sup>1</sup>; Raphael Bruckner<sup>1</sup>; Fana Gebreab<sup>1</sup>; Melanie Gygi<sup>1</sup>; John Szpyt<sup>1</sup>; Stanley Tam<sup>1</sup>; Gabriela Zarraga<sup>1</sup>; Gregory Colby<sup>1</sup>; Kurt Baltier<sup>1</sup>; Rui Dong<sup>2</sup>; Virginia Guarani<sup>1</sup>; Laura Pontano Vaites<sup>1</sup>; Alban Ordureau<sup>1</sup>; Ramin Rad<sup>1</sup>; Brian Erickson<sup>1</sup>; Martin Wuehr<sup>1</sup>; Joel Chick<sup>1</sup>; Bo Zhai<sup>1</sup>; Deepak Kolippakkam<sup>1</sup>; Julian Mintseris<sup>1</sup>; Robert Obar<sup>1</sup>; Tim Harris<sup>3</sup>; Sypros Artavanis-Tsakonas<sup>3</sup>; Mathew Sowa<sup>1</sup>; Pietro DeCamilli<sup>2</sup>; Joao Paulo<sup>1</sup>; J. Wade Harper<sup>1</sup>; Steven Gygi<sup>1</sup>; <sup>1</sup>Harvard Medical School, Boston, MA; <sup>2</sup>Yale School of Medicine, New Haven, CT; <sup>3</sup>Biogen Idec, Cambridge, MA
- MOF am 09:30 **A Sentinel Protein Assay for the Simultaneous Quantification of Cellular Processes;** Martin Soste<sup>1</sup>; Rita Hrabakova<sup>2</sup>; Stefanie Wanka<sup>3</sup>; Andre Melnik<sup>1</sup>; Paul Boersema<sup>1</sup>; Christian von Mering<sup>3</sup>; Paola Picotti<sup>1</sup>; <sup>1</sup>ETH Zurich, Zurich, Switzerland; <sup>2</sup>Academy of Sciences of the Czech Republic, Libechov, Czech Republic; <sup>3</sup>University of Zurich, Zurich, Switzerland
- MOF am 09:50 **Systems Biology Approach Reveals Drug Resistance Mechanism in Multiple Myeloma;** Junmin Peng; *St. Jude Children's Research Hospital, Memphis, TN*
- MOF am 10:10 **Mapping the Sites of Interaction of a Hub Protein in a Transcription Factor Protein Interaction Network using the HaloTag;** Charles Banks; Gina Boanca; Zachary Lee; Laurence Florens; Michael

Washburn; *Stowers Institute for Medical Research, Kansas City, MO*

### 8:30 – 10:30 AM, MONDAY MORNING

#### ENERGY, PETROLEUM, AND BIOFUELS: ADVANCES IN MS DESIGN AND INFORMATICS

**Matthew Hurt (Chevron) presiding**  
Ballroom 222/224

- MOG am 08:30 **Comparison of Atmospheric Solid Analysis Probe with Other Atmospheric Pressure Ionization Sources by Ion Mobility-Mass Spectrometry using PetroOrg Software;** Mathilde Farenc<sup>1,5</sup>; Yuri E. Corilo<sup>2,3</sup>; Priscila M. Lalli<sup>3</sup>; Eleanor Riches<sup>4</sup>; Ryan P. Rodgers<sup>2</sup>; Carlos Afonso<sup>1</sup>; Pierre Giusti<sup>5</sup>; <sup>1</sup>University of Rouen, Mont Saint Aignan, FRANCE; <sup>2</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>3</sup>Future Fuels Institute, Tallahassee, FL; <sup>4</sup>Waters Corporation, Wilmslow, UK; <sup>5</sup>TOTAL Refining and Chemicals, Gonfreville l'Orcher, France
- MOG am 08:50 **Dissociation of Petroleum Components using Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Juan Wei; Simona Gherghel; Mark Barrow; *University of Warwick, Coventry, UK*
- MOG am 9:10 **APCI and APPI-GC/MS-MS for Characterization of the Macondo Crude Oil and the Oil Spill;** Vladislav Lobodin<sup>1,2</sup>; Ryan P. Rodgers<sup>1,2</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>Future Fuels Institute, Tallahassee, FL
- MOG am 09:30 **Alicyclic Structures in Sediments and Kerogens: Potential Sources of Petroleum;** Patrick Hatcher; Blaine Hartman; Nicole Didonato; Derek Waggoner; *Old Dominion University, Norfolk, VA*
- MOG am 09:50 **Algae Biomass Characterization by Traveling Wave Ion Mobility Mass Spectrometry;** Maira Fasciotti<sup>1</sup>; Ingrid Chastinet Ribeiro<sup>1</sup>; Paulo Roque Martins Silva<sup>1</sup>; Thays V. Monteiro<sup>1</sup>; Gustavo H. M. F. Souza<sup>2</sup>; Julia Itacolomy da Silva<sup>1</sup>; Romeu J. Daroda<sup>1</sup>; Valnei S. Cunha<sup>1</sup>; Claudia Maria Luz Lapa Teixeira<sup>3</sup>; Amarjit S. Sarpal<sup>1</sup>; <sup>1</sup>INMETRO, Duque De Caxias, Brazil; <sup>2</sup>Waters Cooperation, Rio de Janeiro, Brazil; <sup>3</sup>National Institute of Technology, INT, Rio de Janeiro, Brazil
- MOG am 10:10 **Identification of the Phenol Functionality in Monomeric Lignin Degradation Products via Negative Ion-Molecule Reactions with Diethylmethoxyborane;** Hanyu Zhu; Hilikka Kenttämä; *Purdue University, West Lafayette, IN*

### 8:30 – 10:30 AM, MONDAY MORNING

#### ADVANCES IN SOFTWARE AND HARDWARE TO IMPROVE DMPK WORKFLOWS

**Hongying Gao (Pfizer, Inc.) presiding**  
Ballroom 220/221

- MOH am 08:30 **Automated LC/MS Quantitation Method Development Using a Hybrid Quadrupole-Orbitrap Mass Spectrometer;** Jonathan L. Josephs; Keeley Murphy; Hongxia (Jessica) Wang; David Brant; Jamie K Humphries; Kristi Akervik; Nicholas Duczak, Jr; Mark Sanders; *Thermo Fisher Scientific, San Jose, CA*
- MOH am 08:50 **Utilization of MassMetaSite for in vitro and in vivo Metabolite Identification of Complex Therapeutic Peptides;** Heather Trexler<sup>1</sup>; Kevin Bateman<sup>1</sup>; Richard Gundersdorf<sup>1</sup>; Fabien Fontaine<sup>2</sup>; Rodger Tracy<sup>1</sup>; Kenneth Koeplinger<sup>1</sup>; Ismael Zamora<sup>2</sup>; Mark Cancilla<sup>1</sup>; <sup>1</sup>Merck & Co., West Point, PA; <sup>2</sup>Lead Molecular Design, S.L., Sant Cugat Del Valles, Spain

## MONDAY MORNING AND AFTERNOON ORAL SESSIONS



MOH am 09:10 **Fully Integrated Novel IMS-QToF Informatics Platform for Rapid Drug Screening and Elucidation;** Russell Mortishire-Smith<sup>1</sup>; Jayne Kirk<sup>1</sup>; Nick Tomczyk<sup>1</sup>; Martin Palmer<sup>1</sup>; Richard Denny<sup>1</sup>; Alan Prile<sup>1</sup>; Simon Cubbon<sup>1</sup>; Yun Alelyunas<sup>2</sup>; Mark Wrona<sup>2</sup>; <sup>1</sup>*Waters MS Technologies, Wilmslow, UK*; <sup>2</sup>*Waters Corporation, Milford, MA*

MOH am 09:30 **A Novel Platform for Automated High-Throughput LC-MS/MS Analysis of *In Vitro* ADME and *In Vivo* ADME PK Samples;** Andreas Luippold; Wolfgang Joerg; Klaus Klinder; Daniel Bischoff; *Boehringer Ingelheim Pharma GmbH & Co KG, Biberach, GERMANY*

MOH am 09:50 **Untargeted and Rapid Detection and Characterization of Modified Monoclonal Antibodies using LC-TripleTOF and Multivariate Statistical Analysis;** Ming Yao<sup>1</sup>; Xu Wang<sup>2</sup>; Weiping Zhao<sup>1</sup>; Li Ma<sup>1</sup>; John T. Mehl<sup>1</sup>; Yi Zhang<sup>2</sup>; Sahana Mollah<sup>2</sup>; W. Griff Humphreys<sup>1</sup>; Mingshe Zhu<sup>1</sup>;

<sup>1</sup>*Bristol-Myers Squibb, Princeton, NJ*; <sup>2</sup>*AB SCIEX, Framingham, MA*

MOH am 10:10 **Advances in HRMS and *in vitro* Systems Provide an Option to Detect and Characterize Human Disproportionate Metabolites of Loratadine;** Ragu Ramanathan<sup>1</sup>; Cornelia Smith<sup>2</sup>; Lakshmi Ramanathan<sup>2</sup>; Caroline Lee<sup>3</sup>; Helen Shen<sup>2</sup>; Zamas Lam<sup>2</sup>; <sup>1</sup>*Pfizer, Groton, CT*; <sup>2</sup>*QPS, Newark, DE*; <sup>3</sup>*Ardea Biosciences, San Diego, CA*

10:30 AM – 2:30 PM, MONDAY  
MONDAY POSTER SESSION  
Poster/Exhibit Hall  
Lunch concessions are open 11:00 am – 2:00 pm

11:30 am – 1:00 pm  
Undergraduate Students  
Meet the Experts at tables reserved for you.

## MONDAY AFTERNOON ORAL SESSIONS

2:30 – 4:30 PM, MONDAY AFTERNOON  
ION MOBILITY, FAIMS & DMS:  
NEW DEVELOPMENTS AND APPLICATIONS  
Melvin Park (Bruker Daltonics, Inc.) presiding  
Hall 5

MOA pm 2:30 **Very Long Path Length High Resolution Ion Mobility Separations using Structures for Lossless Ion Manipulations (SLIM);** Richard D. Smith; Ian K. Webb; Ahmed Hamid; Sandilya V. B. Garimella; Yehia M. Ibrahim; Aleksey V. Tolmachev; Spencer A. Prost; Gordon A. Anderson; Erin S. Baker; *Pacific Northwest National Laboratory, Richland, WA*

MOA pm 2:50 **3D Printed Concentric Ring Drift Tube with Nanoelectrospray Ionization Source for ion Focusing, Separation, and Detection under Ambient Conditions;** Zane Baird; Adam Hollerbach; R. Graham Cooks; *Purdue University, West Lafayette, IN*

MOA pm 3:10 **Improvement of Resolution and Peak Capacity for Differential Ion Mobility Spectrometry Scans using Linked Helium and Compensation Field Scans;** Brandon G. Santiago; Rachel A. Harris; Gary L. Glish; *The University of North Carolina at Chapel Hill, Chapel Hill, NC*

MOA pm 3:30 **A Polarizable Projection Approximation Method to Predict Molecular Cross Section for Use in Ion Mobility / Mass Spectrometry Studies.;** Christian Bleiholder; *Florida State University, Tallahassee, FL*

MOA pm 3:50 **Differential Photofragmentation Patterns for Mobility Selected Glycans;** Kelsey A. Morrison; Enamul H. Khan; Brian H. Clowers; *Washington State University, Pullman, WA*

MOA pm 4:10 **Coupling FAIMS and LESA for the Analysis of Proteins Directly from Biological Substrates ;** Andrew Creese<sup>1</sup>; Joscelyn Sarsby<sup>1</sup>; Rian Griffiths<sup>1</sup>; Elizabeth Randall<sup>1</sup>; Alan Race<sup>2</sup>; Josephine Bunch<sup>2</sup>; Helen Cooper<sup>1</sup>; <sup>1</sup>*University of Birmingham, Birmingham, United Kingdom*; <sup>2</sup>*The National Physical Laboratory, Teddington, N/A*

2:30 – 4:30 PM, MONDAY AFTERNOON  
INFORMATICS: METABOLOMICS  
Alexey Nesvizhskii (University of Michigan) presiding  
Room 130/132

MOB pm 2:30 **Accurate Mass for Improved Metabolite Identification via High-Resolution GC/MS;** Nicholas W. Kwiecien; Derek J. Bailey; Matthew J. P. Rush; Arne Ulbrich; Alexander S. Hebert; Michael S. Westphall; Joshua J. Coon; *University of Wisconsin, Madison, WI*

MOB pm 2:50 **Exploring Correlation Networks for the Analysis of Metabolomics Data;** Alla Karnovsky<sup>1</sup>; Sumanta Basu<sup>2</sup>; Bill Duren<sup>1</sup>; Charles Evans<sup>1</sup>; George Michailidis<sup>1</sup>; Charles Burant<sup>1</sup>; <sup>1</sup>*University of Michigan, Ann Arbor, MI*; <sup>2</sup>*University of California, Berkeley, CA*

MOB pm 3:10 **Improving the Efficiency of Feature Annotation in Untargeted Metabolomics: Integrating Metabolic Pathway Analysis with XCMS and METLIN;** Anna Chen<sup>1,2</sup>; Rebecca Schugar<sup>3</sup>; Peter Crawford<sup>4</sup>; Gary Patti<sup>1,2</sup>; <sup>1</sup>*Washington University in St. Louis, St. Louis, MO*; <sup>2</sup>*Washington University Medical School, St. Louis, MO*; <sup>3</sup>*Cleveland Clinic Lerner Research Institute, Cleveland, OH*; <sup>4</sup>*Sanford-Burnham Medical Research Institute, Orlando, FL*

MOB pm 3:30 **Constructing MS<sup>n</sup> Mass Spectral Library for More Accurate Metabolite Identification;** Xiaoyu Yang; Pedatsur Neta; Yuxue Liang; Stephen Stein; *NIST, Gaithersburg, MD*

MOB pm 3:50 **Greazy: Open-Source Software for Automated Phospholipid MS/MS Identification;** Michael Koehen<sup>1</sup>; Matthew Chambers<sup>1</sup>; Jerry Holman<sup>1</sup>; Thomas Metz<sup>2</sup>; Alexey Nesvizhskii<sup>3</sup>; Susan T. Weintraub<sup>4</sup>; David Tabb<sup>1</sup>; <sup>1</sup>*Vanderbilt University, Nashville, TN*; <sup>2</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>3</sup>*University of Michigan, Ann Arbor, MI*; <sup>4</sup>*Univ. of Texas HSC, San Antonio, TX*

MOB pm 4:10 **Translating Molecular Information from HR Imaging MS data: towards Spatial Annotation of the Cellular Metabolome;** Andrew D. Palmer<sup>1,2</sup>; Eric Weaver<sup>3</sup>; Marco Hennrich<sup>1</sup>; Jens Fuchser<sup>4</sup>; Michael Becker<sup>4</sup>; Anne-Claude Gavin<sup>1</sup>; Amanda B. Hummon<sup>3</sup>; Theodore Alexandrov<sup>1,5</sup>; <sup>1</sup>*EMBL Heidelberg, Heidelberg, Germany*; <sup>2</sup>*University of Bremen, Bremen, Germany*; <sup>3</sup>*University of Notre Dame, Notre Dame, IN*; <sup>4</sup>*Bruker Daltonik GmbH, Bremen, Germany*; <sup>5</sup>*SCILS, Bremen, Germany*

## MONDAY AFTERNOON ORAL SESSIONS

### 2:30 – 4:30 PM, MONDAY AFTERNOON

#### TOP-DOWN PROTEIN ANALYSIS

**Mark McComb (Boston University School of Medicine) presiding**  
Room 123/124

- MOC pm 2:30 **Stochastic SILAC for Intact Protein Quantitation in Any Organism Using Any Growth Medium or Feed**; Jared R. Auclair; Joseph Salisbury; Jeniffer Quijada; Jeffrey Agar; *Northeastern University, Boston, MA*
- MOC pm 2:50 **Characterizing Protein Complexes and Mapping their Surface and Interfacial Residues in One Native Top-Down MS Experiment with FTICR**; Huilin Li; Rachel R. Ogorzalek Loo; Joseph A. Loo; *University of California, Los Angeles, Los Angeles, CA*
- MOC pm 3:10 **Detailed Characterisation of Photoactivatable Metalloprotein Interactions with Peptides, Proteins, and DNA by High Resolution Tandem FT-ICR MS**; Christopher A. Wootton; Andrea F. Lopez-Clavijo; Evyenia Shaili; Mark P. Barrow; Peter J. Sadler; Peter B. O'Connor; *University of Warwick, Coventry, UK*
- MOC pm 3:30 **Top-Down Proteogenomics of Pathogenic *Helicobacter***; Egor Vorontsov<sup>1,2</sup>; Frédéric Fischer<sup>1</sup>; Christian Malosse<sup>1,2</sup>; Hilde de Reuse<sup>1</sup>; Julia Chamot-Rooke<sup>1,2</sup>; *<sup>1</sup>Institut Pasteur, Paris, France; <sup>2</sup>CNRS, Paris, France*
- MOC pm 3:50 **Integrated Proteogenomic Analysis of CompRef Breast Tumor Xenografts via Top-Down and Bottom-Up Proteomics**; Ioanna Ntai<sup>1</sup>; Richard Leduc<sup>1</sup>; Ryan Fellers<sup>1</sup>; Petra Erdmann-Gilmore<sup>2</sup>; Sherri Davies<sup>2</sup>; Jeanne Rumsey<sup>2</sup>; Bryan Early<sup>1</sup>; Paul Thomas<sup>1</sup>; Shunqiang Li<sup>2</sup>; Philip Compton<sup>1</sup>; Matthew Ellis<sup>3</sup>; Kelly Ruggles<sup>4</sup>; David Fenyo<sup>5</sup>; Emily Boja<sup>6</sup>; Henry Rodriguez<sup>6</sup>; Reid Townsend<sup>2</sup>; Neil Kelleher<sup>1</sup>; *<sup>1</sup>Northwestern University, Evanston, IL; <sup>2</sup>Washington University School of Medicine, St. Louis, Missouri; <sup>3</sup>Baylor College of Medicine, Houston, TX; <sup>4</sup>NYU Langone Medical Center, New York, NY; <sup>5</sup>New York University, New York, NY; <sup>6</sup>National Cancer Institute, Bethesda, MD*
- MOC pm 4:10 **Intact Protein Profiling: On the Hunt for Wound Healing Factors**; Giuseppe Infusini<sup>1</sup>; Condina Mark<sup>2</sup>; Jemma Evans<sup>3</sup>; Lois Salamonsen<sup>3</sup>; Andrew Webb<sup>1</sup>; *<sup>1</sup>Walter & Eliza Hall Institute, Parkville, Australia; <sup>2</sup>Bruker, Preston, Australia; <sup>3</sup>MIMR-PHI, Clayton, Australia*

### 2:30 – 4:30 PM, MONDAY AFTERNOON

#### PLANT-OMICS

**A. Daniel Jones (Michigan State University) presiding**  
Room 120/127

- MOD pm 2:30 **A Family-Wide Phosphoproteomic Study of Leucine-Rich Repeat Receptor-Like Kinase Autophosphorylation in *Arabidopsis thaliana***; Srijeet Mitra<sup>1</sup>; Ruiqiang Chen<sup>1</sup>; Murali Dhundaydham<sup>1</sup>; Xiaofeng Wang<sup>1</sup>; Kevin Blackburn<sup>1</sup>; Uma Kota<sup>1</sup>; Michael Goshe<sup>1</sup>; Daniel Schwartz<sup>2</sup>; Steven Huber<sup>3</sup>; Steven Clouse<sup>1</sup>; *<sup>1</sup>North Carolina State University, Raleigh, NC; <sup>2</sup>University of Connecticut, Storrs, CT; <sup>3</sup>University of Illinois, Urbana, IL*
- MOD pm 2:50 **Rapid and Comprehensive Proteome Profiling in Plants**; Catherine Minogue; Alicia Richards; Harald Marx; Dhileepkumar Jayaraman; Junko Maeda; Shanmugam Rajasekar; Michael S. Westphall; Michael R. Sussman; Jean-Michel Ane; Joshua J. Coon; *University of Wisconsin, Madison, WI*
- MOD pm 3:10 **Metabolic Interplay between the Asian Citrus Psyllid and its *Proffella* Symbiont: An Achilles' Heel of the Citrus Greening Insect Vector**; Michelle Cilia<sup>1,2</sup>; John Ramsey<sup>3</sup>; Richard S. Johnson<sup>4</sup>; Jason Hoki<sup>3</sup>; David Hall<sup>5</sup>; Frank

Schroeder<sup>3</sup>; Michael J. MacCoss<sup>4</sup>; *<sup>1</sup>United States Department of Agriculture, ARS, Ithaca, NY;*

*<sup>2</sup>Department of Plant Pathology, Cornell University, Ithaca, NY; <sup>3</sup>Boyce Thompson Institute for Plant Research, Ithaca, NY; <sup>4</sup>Univ of Washington, Seattle, WA; <sup>5</sup>United States Department of Agriculture, ARS, Fort Pierce, FL*

- MOD pm 3:30 **Integrating Multiple -omic Resources to Better Characterize Photosynthetic Diversity in Constitutive and Facultative Crassulacean Acid Metabolism Plants**; Paul Abraham<sup>1</sup>; Hengfu Yin<sup>3</sup>; Timothy Tschaplinski<sup>1</sup>; Gerald Tuskan<sup>1</sup>; Xiaohan Yang<sup>1</sup>; Bernard W. M. Wone<sup>2</sup>; Won Cheol Yim<sup>2</sup>; Karen A. Schlauch<sup>2</sup>; John C. Cushman<sup>2</sup>; Robert Hettich<sup>1</sup>; *<sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>University of Nevada, Reno, NV; <sup>3</sup>Chinese Academy of Forestry, Zhejiang, China*
- MOD pm 3:50 **Using Mass Spectrometry-Based Metabolomics for Chemotaxonomy Studies**; Dominique Ardura; Oliver Fiehn; *Genome Center, University of California, Davis, CA*
- MOD pm 4:10 **Chemical Isotope Labeling LC-MS for Profiling Spatial Distribution of Metabolites in Ginseng Roots**; Chiao-Li Tseng; Liang Li; *University of Alberta, Edmonton, Canada*

### 2:30 – 4:30 PM, MONDAY AFTERNOON

#### CLINICAL DIAGNOSTICS

**Christine Snozek (Mayo Clinic) presiding**  
Theater

- MOE pm 2:30 **Personalized Detection of Multiple Myeloma Tumor Burden**; Melissa Hoffman; Saavedra-Roman Luis; Sean Yoder; Rachid Baz; Kaaron Benson; Aunshka Collins; Robert Sprung; Jamie Teer; John Koomen; *Moffitt Cancer Center, Tampa, FL*
- MOE pm 2:50 **Cerebrospinal Fluid Tau Phosphopeptides: Detection, Quantitative Analysis and Assessment for the Diagnosis of Neurological Diseases**; Nicolas R Barthélemy<sup>1,5</sup>; Christophe Hirtz<sup>1</sup>; Martial Seveno<sup>3</sup>; Susanna Schraen-Maschke<sup>2</sup>; Randall J Bateman<sup>5</sup>; Audrey Gabelle<sup>1</sup>; François Becher<sup>4</sup>; Philippe Marin<sup>3</sup>; Sylvain Lehmann<sup>1</sup>; *<sup>1</sup>LBPC, IRMB, CHU Montpellier St. Eloi, Montpellier, France; <sup>2</sup>Inserm, UMR 837, IMPRT, Lille, France; <sup>3</sup>PPF, IGF, CNRS-UMR 5203, Inserm U661, Montpellier, France; <sup>4</sup>CEA, IBI Tec-S, SPI, LEMM, Gif-sur-Yvette, France; <sup>5</sup>Washington University School of Medicine, St. Louis, MO*
- MOE pm 3:10 **MALDI Imaging Classification of Tumors in Formalin-Fixed Paraffin-Embedded Tissues**; Rita Casadonte<sup>1</sup>; Mark Kriegsmann<sup>2</sup>; Jan Hendrik Kobarg<sup>3</sup>; Dennis Trede<sup>3</sup>; Michael Becker<sup>4</sup>; Peter Maaß<sup>5</sup>; Sören-Oliver Deininger<sup>4</sup>; Katrin Friedrich<sup>6</sup>; Daniela Aust<sup>6</sup>; Christian Pilarsky<sup>6</sup>; Gustavo Baretton<sup>6</sup>; Mike Otto<sup>1,7</sup>; Jörg Kriegsmann<sup>7</sup>; *<sup>1</sup>Proteopath GmbH, Trier, Germany; <sup>2</sup>University of Heidelberg, Heidelberg, Germany; <sup>3</sup>SCI LS GmbH, Bremen, Germany; <sup>4</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>5</sup>University of Bremen, Bremen, Germany; <sup>6</sup>University of Dresden, Dresden, Germany; <sup>7</sup>Center for Histology, Cytology and Molecular Diagn, Trier, Germany*
- MOE pm 3:30 **Analysis of Urinary Free Oligosaccharides for the Diagnosis of Lysosomal Storage Diseases using UPLC-SRM**; Rongrong Huang; Tim Wood; *Greenwood Genetic Center, Greenwood, SC*
- MOE pm 3:50 **MALDI-TOF Analysis of Whole Blood: Its Usefulness and Potential in the Assessment of HbA1c Levels in Diabetes Mellitus**; Stephen J. Hattan<sup>1</sup>; Kenneth Parker<sup>1</sup>; Marvin Vestal<sup>1</sup>; David Herold<sup>3</sup>; Jane Yang<sup>4</sup>; Mark W Duncan<sup>2</sup>; *<sup>1</sup>SimulTOF/*



VIC Instruments, Sudbury, MA; <sup>2</sup>Univ. Colorado, School of Medicine, AURORA, CO; <sup>3</sup>VAMC/ UCSD, San Diego, CA; <sup>4</sup>UCSD, San Diego, CA

MOE pm 4:10 **Clinical Diagnostics of Rare Kidney Disease with UPLC-MS/MS; Finnur Eiriksson<sup>1,2</sup>; Hrafnhildur Runoldsdottir<sup>1</sup>; Vidar O. Edvardsson<sup>3</sup>; Runolfur Palsson<sup>1,3</sup>; Margret Thorsteinsdottir<sup>1,2</sup>; <sup>1</sup>University of Iceland, Reykjavik, Iceland; <sup>2</sup>ArcticMass, Reykjavik, Iceland; <sup>3</sup>Landspítali, Reykjavik, Iceland**

**2:30 – 4:30 PM, MONDAY AFTERNOON  
PTMS: ADVANCES IN ISOLATION, ENRICHMENT,  
DERIVATIZATION AND SEPARATION**

**Erik Soderblom (Duke University School of Medicine) presiding  
Room 106**

MOF pm 2:30 **PTM Profiling in Serum & Plasma to Identify Potential Biomarkers by Immunoaffinity LC-MS Methods; Hongbo Gu; Jian Min Ren; Jeffrey Silva; Cell Signaling Technology, Danvers, MA**

MOF pm 2:50 **Optimization of Automated Phosphopeptide Enrichment using Fe<sup>3+</sup>-NTA IMAC on the Bravo AssayMAP Liquid Handling Robotics Platform; Jennifer Abelin<sup>1</sup>; Caitlin Feeney<sup>1</sup>; Jinal Patel<sup>1</sup>; Lola Fagbami<sup>1</sup>; Xiaodong Lu<sup>1</sup>; Daniel Lam<sup>1</sup>; Jason Russell<sup>2</sup>; Steve Murphy<sup>2</sup>; Gavin Fischer<sup>2</sup>; Steven A. Carr<sup>1</sup>; Jacob D. Jaffe<sup>1</sup>; <sup>1</sup>Broad Institute of MIT and Harvard, Cambridge, MA; <sup>2</sup>Agilent Technologies, Inc., Madison, WI**

MOF pm 3:10 **Quantifying Reversible Oxidation of Protein Thiols in Photosynthetic Organisms; William Slade<sup>1</sup>; Emily Werth<sup>1</sup>; Evan McConnell<sup>1</sup>; Sophie Alvarez<sup>2</sup>; Leslie Hicks<sup>1</sup>; <sup>1</sup>University of North Carolina, Chapel Hill, NC; <sup>2</sup>Danforth Center, St Louis, MO**

MOF pm 3:30 **An Integrated Workflow for Enrichment, Separation, and Quantitation of Plasma Glycoproteins in Prostate Cancer and Benign Prostate Hyperplasia; Sarah Totten; Majlinda Kullolli; Cheylene Tanimoto; James Brooks; Sharon Pitteri; Stanford University School of Medicine, Palo Alto, CA, USA**

MOF pm 3:50 **Isobaric Labeling Enables 10-Plex Quantitative Analysis Of Ubiquitylated Peptides: A Diagnostic Ion to Improve Identification and Quantification; Christopher M. Rose<sup>1</sup>; Marta Isasa<sup>1</sup>; Sean A. Beausoleil<sup>2</sup>; Steven P. Gygi<sup>1</sup>; <sup>1</sup>Harvard Medical School, Boston, MA; <sup>2</sup>Cell Signaling Technology, Danvers, MA**

MOF pm 4:10 **A New Method for Enhanced Identification of Citrullinated Peptides using SWATH-MS Technology; Ronald Holewinski; Justyna Fert-Bober; Jennifer Van Eyk; Cedars Sinai Medical Center, Los Angeles, CA**

**2:30 – 4:30 PM, MONDAY AFTERNOON  
IMAGING: BIOMEDICAL APPLICATIONS**

**Jihyeon Lim (Albert Einstein College of Medicine) presiding  
Ballroom 222/224**

MOG pm 2:30 **Direct Structure-Specific Quantitative Molecular Imaging of Neurotransmitters in Experimental Parkinson's Disease; Mohammadreza Shariatgorji<sup>1</sup>; Anna Nilsson<sup>1</sup>; Patrik Källback<sup>1</sup>; Erwan Bezdard<sup>3</sup>; Per Svenningsson<sup>2</sup>; Per E. Andren<sup>1</sup>; <sup>1</sup>Uppsala University, Uppsala, Sweden; <sup>2</sup>Karolinska Institutet, Stockholm, Sweden; <sup>3</sup>Université de Bordeaux, Bordeaux, France**

MOG pm 2:50 **Glycopathology and Glycoimmunology of Prostate Cancer Tissues by N-Glycan MALDI Mass Spectrometry Imaging; Richard R Drake; Ellen Jones; Thomas Powers; Medical University of South Carolina, Charleston, SC**

MOG pm 3:10 **Anatomy-guided Differential Analysis of Imaging Mass Spectrometry Data Using the Allen Mouse**

**Brain Atlas; Nico Verbeeck<sup>1,2</sup>; Jeffrey Spraggins<sup>4</sup>; Junhai Yang<sup>4</sup>; Bart De Moor<sup>1,2</sup>; Richard M. Caprioli<sup>4</sup>; Etienne Waelkens<sup>5,6</sup>; Raf Van de Plas<sup>3,4</sup>; <sup>1</sup>ESAT-STADIUS, KU Leuven, Leuven, Belgium; <sup>2</sup>iMinds Medical IT, Leuven, Belgium; <sup>3</sup>Delft University of Technology, Delft, Netherlands; <sup>4</sup>Vanderbilt University, Nashville, TN; <sup>5</sup>Dept. Cellular and Molecular Medicine, KU Leuven, Leuven, Belgium; <sup>6</sup>Sybioma, Leuven, Belgium**

MOG pm 3:30 **Application of MALDI-MSI to Identify Biomarkers of Radiation-Induced Lung Injury and Medical Countermeasure Development; Claire L. Carter; Jace W. Jones; Isabel L. Jackson; Zeljko Vujaskovic; Sean Kearney; Kory Barrow; Kaitlyn Kieta; Cheryl Taylor-Howell; Allison Gibbs; Ann M. Farese; Thomas J. MacVittie; Maureen A. Kane; University of Maryland, Baltimore, MD**

MOG pm 3:50 **Tools for Multivariate Analysis (MVA) of 2D and 3D Mass Spectrometry Images; Daniel Graham; Lara Gamble; Department of Bioengineering, UW, Seattle, Washington**

MOG pm 4:10 **Phospholipid MALDI Imaging Mass Spectrometry Stratification of Colorectal Cancer Liver Metastasis Clinical Biopsies; Heath Patterson<sup>1</sup>; Balqis Alabdulkarim<sup>2</sup>; Aurélien Thomas<sup>3</sup>; Martin M. Marcinkiewicz<sup>4</sup>; Anthoula Lazaris<sup>2</sup>; Peter Metrakos<sup>2</sup>; Pierre Chaurand<sup>1</sup>; <sup>1</sup>Dept. of Chemistry, University of Montreal, Montreal, Quebec, Canada; <sup>2</sup>Dept. of Surgery, McGill University, Montreal, Quebec, Canada; <sup>3</sup>Unit of Toxicology, CURML, University of Lausanne, Lausanne, Switzerland; <sup>4</sup>Cytochem Inc., Montreal, Quebec, Canada**

**2:30 – 4:30 PM, MONDAY AFTERNOON  
QUANTITATIVE ANALYSIS IN DRUG DISCOVERY FOR  
SMALL MOLECULES**

**Rick King (PharmaCadence Analytical Services) presiding  
Ballroom 220/221**

MOH pm 2:30 **The Evaluation and Development of Automated Workflows in Blood, Plasma and Urine Using Volumetric Absorptive Microsampling (VAMS); Leanne Grafmuller; Joseph Tweed; Zhenhua Gu; Mark Wallace; Mark Milisci; Rick Steenwyk; Ragu Ramanathan; Pfizer, Groton, CT**

MOH pm 2:50 **Calibration Curve Sensitivity: The Role of Internal Standard on Slope and Precision of Clinical LC-MS/MS Assays; Brian Rappold; Andrew Lickteig; Matthew Salske; Essential Testing, Collinsville, IL**

MOH pm 3:10 **LC-MS/MS and LC-HRMS Approaches to Support Toxicity Studies of a Glycolipid Vaccine Adjuvant; Kasie Fang; Chester L. Bowen; Jonathan Kehler; Kendal Ryter; GlaxoSmithKline, King of Prussia, PA**

MOH pm 3:30 **Improving Quantitative Analysis through Reduction of Matrix Suppression Effects by coupling Multi-Dimensional Chromatography to ESI-MS; Tom Van De Goor; Stephan Buckenmaier; Agilent Technologies, Waldbronn, GERMANY**

MOH pm 3:50 **Whole blood Analysis using New Solid Phase Microextraction Devices and Investigation of the Hematocrit Effect; Nathaly Reyes Garces; Barbara Bojko; Janusz Pawliszyn; University of Waterloo, Waterloo, CANADA**

MOH pm 4:10 **Comparison of Travelling Wave IMS-QToF Geometries and Acquisition Modes for Quantitative Analysis; Mark Wrona<sup>1</sup>; Yun Aielyunas<sup>1</sup>; Jayne Kirk<sup>2</sup>; Martin Palmer<sup>2</sup>; Nick Tomczyk<sup>2</sup>; Russell Mortishire-Smith<sup>2</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Waters MS Technologies, Wilmslow, United Kingdom**

## MONDAY AFTERNOON AND TUESDAY MORNING ORAL SESSIONS

4:45 – 5:30 PM, MONDAY AFTERNOON  
AWARD LECTURE

Jenny Brodbelt (University of Texas, Austin) presiding  
Hall 5



**Award for a Distinguished Contribution  
in Mass spectrometry**

**Brian T. Chait**  
The Rockefeller University

5:45 – 7:00 PM, MONDAY AFTERNOON  
WORKSHOPS  
There are light refreshments in the common areas.

01. Has Photoionization Reached its Potential? Focus on APPI, Room 130
02. Enabling proteomics informatics on the Amazon cloud, Room 131
03. Advanced MS and separation approaches for biofuels and petroleum, Room132

04. The Galaxy Framework for MS-based Informatics, Room 123/124
05. Defining Resolution in Imaging MS - A Quest for Solid Ground, Room 120/127
06. Ion Trap Interest Group: new experiments and old tricks, Room 260/267
07. Metal Cationization of Biomolecules and its Analytical Applications, Room 274
08. Methods and Tools for Intra- and Inter-Experiment LC MS Performance Tracking, Room 275
09. Challenges and progress towards the site-specific characterization of glycoprotein heterogeneity, Room 230
10. Mass Spectrometry Applications in Art, cultural Heritage, and Natural History, Room 231
11. More DMPK Knowledge from Less Sample: Leveraging Modern LC-MS Instruments for Small Sample Amounts, Room 232
12. Metabolomics: Emerging Technologies for Continued Innovation, Ballroom 222/224
13. Which Career Path is Right for Me? - Young Mass Spectrometrists Workshop, Ballroom 220/221

AFTER 8:00 PM  
CORPORATE HOSPITALITY SUITES  
RENAISSANCE GRAND HOTEL

## TUESDAY MORNING ORAL SESSIONS

8:30 – 10:30 AM, TUESDAY MORNING  
INSTRUMENTATION: TIME-OF-FLIGHT AND QTOF  
Jody C. May (Vanderbilt University) presiding  
Hall 5

- TOA am 08:30 **High Resolution Multi-Reflecting TOFMS with Multiplexing by Encoded Frequent Pulsing for Increasing the Duty Cycle 10-100 Times;** Peter Willis<sup>1</sup>; Viatcheslav Artaev<sup>1</sup>; George Tikhonov<sup>1</sup>; Kevin Siek<sup>1</sup>; Vasily Makarov<sup>2</sup>; Anatoly Verenchikov<sup>2</sup>; <sup>1</sup>LECO Corporation, St Joseph, MI; <sup>2</sup>MSC-CG, Bar, Montenegro
- TOA am 08:50 **Novel Operating Modes of an Ion Mobility Quadrupole Time-Of-Flight Hybrid Instrument;** Jason L Wildgoose; Kevin Giles; Keith Richardson; Steven Pringle; *Waters Corporation, Manchester, UK*
- TOA am 09:10 **A W-geometry ortho-TOF MS with High Resolution and Up To 100% Duty Cycle for MS/MS;** Samuel Merenbloom<sup>1</sup>; Nic Bloomfield<sup>1</sup>; Alexandre Loboda<sup>2</sup>; Igor Chernushevich<sup>1</sup>; <sup>1</sup>SCIEX, Concord, Canada; <sup>2</sup>Fluidigm Canada Inc., Markham, Canada
- TOA am 09:30 **Inductively Coupled Plasma Distance-Of-Flight Mass Spectrometry with an ionCCD Camera detector;** Elise Dennis<sup>1</sup>; Steven J. Ray<sup>1</sup>; Christie G. Enke<sup>2</sup>; Charles J. Barinaga<sup>3</sup>; David W. Koppenaal<sup>3</sup>; Gary M. Hieftje<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN; <sup>2</sup>University of New Mexico, Placitas, NM; <sup>3</sup>Pacific NW Nat'l Laboratory, Richland, WA
- TOA am 09:50 **A New Instrument for High Speed, True Pixel and Large Dataset MALDI TOF Imaging;** Jens Höhndorf; Andreas Haase; Arne Fütterer; Michael Becker; Armin Holle; *Bruker Daltonik GmbH, Bremen, Germany*
- TOA am 10:10 **Artificial Intelligent Algorithm, Particle Swarm Optimization (SWARM), Opens a New Era for Mass Spectrometer Application Tune;** Huy Bui<sup>1</sup>; Christian Klein<sup>1</sup>; Dorothy Yang<sup>1</sup>; Yevgeny Kaplun<sup>1</sup>; Syed Lateef<sup>1</sup>; Gregor Overney<sup>1</sup>; Koen Sandra<sup>2</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>Research Institute for Chromatography, Kortrijk, Belgium

8:30 – 10:30 AM, TUESDAY MORNING  
INFORMATICS: MULTI-OMICS INTEGRATION  
Akhilesh Pandry (Johns Hopkins University) presiding  
Room 130/132

- TOB am 08:30 **STATegra – Studying B-Cell Differentiation by Combination of Multiple Omics Datasets;** The STATegra Consortium; Andreas Schmidt; Axel Imhof; *ZFP - LMU Munich, Munich, GERMANY*
- TOB am 08:50 **The Quest for Novel Proteoforms: Integration of Proteomics and Ribosome Profiling Based Translatomics;** Jeroen Crappé; Volodimir Olexiouk; Daria Gawron; Elvis Ndah; Sandra Steyaert; Alexander Koch; Steven Verbruggen; Ellen De Meester; Sarah De Keulenaer; Petra Van Damme; Gerben Menschaert; *Ghent University, Gent, Belgium*
- TOB am 09:10 **Peptide Search Engine Approach for the Detection Of Translated Mutations Based on Sequencing Data, Mutation Databases and Exhaustive Codon Changes;** Pavel Sinitcyn; Stefka Tyanova; Matthias Mann; Juergen Cox; *Max-Planck-Institute of Biochemistry, Martinsried, Germany*
- TOB am 09:30 **Enosi: A web-accessible Proteogenomic Pipeline for Identification of Proteomic Event using Large-scale NGS Data;** Seong Won Cha; Sunghee Woo; Vineet Bafna; *University of California, San Diego, La Jolla, CA*
- TOB am 09:50 **SearchGUI and PeptideShaker Deployed in the Galaxy Framework: A Powerful Informatics Platform for Protein Identification and Beyond;** Ira Cooke<sup>1</sup>; Bjoern Groening<sup>2</sup>; Harald Barsnes<sup>3</sup>; Marc Vaudel<sup>3</sup>; Lennart Martens<sup>4</sup>; James Johnson<sup>6</sup>; Candace Guerrero<sup>5</sup>; Getiria Onsongo<sup>5</sup>; John Chilton<sup>7</sup>; Pratik Jagtap<sup>8</sup>; Tim Griffin<sup>5</sup>; <sup>1</sup>La Trobe University, Melbourne, Australia; <sup>2</sup>University of Freiburg, Freiburg, Germany; <sup>3</sup>University of Bergen, Bergen, Norway; <sup>4</sup>Ghent University, Ghent, Belgium; <sup>5</sup>University of Minnesota, Minneapolis, MN; <sup>6</sup>University of Minnesota Supercomputing Institute, Minneapolis, MN; <sup>7</sup>Pennsylvania State



University, State College, PA; <sup>8</sup>Center for Mass Spectrometry and Proteomics, UMN, St. Paul, MN  
 TOB am 10:10 **Mass Spectrometry Centric Analysis of Public Proteomic Data in ProteomicsDB**; Mathias Wilhelm<sup>1</sup>; Hans-Christian Ehrlich<sup>2</sup>; Judith Schlegl<sup>3</sup>; Wilhelm Becker<sup>2</sup>; Lars Rueckert<sup>2</sup>; **Hannes Hahne**<sup>1</sup>; Bernhard Kuster<sup>1</sup>; <sup>1</sup>Technical University Munich, Freising, GERMANY; <sup>2</sup>SAP SE, Innovation Center Potsdam, Potsdam, Germany; <sup>3</sup>SAP SE, Walldorf, Germany

**8:30 – 10:30 AM, TUESDAY MORNING  
 IMAGING: INSTRUMENTATION AND METHOD**  
**Gary Van Berkel (Oak Ridge National Laboratory) presiding  
 Room 123/124**

TOC am 08:30 **Constant-Distance Mode for High-Resolution Ambient Imaging Using Nanospray Desorption Electrospray Ionization Mass Spectrometry**; **Julia Laskin**<sup>1</sup>; Ingela Lanekoff<sup>2</sup>; Andrey Liyu<sup>1</sup>; Mathew Thomas<sup>1</sup>; <sup>1</sup>Pacific NW National Laboratory, Richland, WA; <sup>2</sup>Uppsala University, Uppsala, SWEDEN  
 TOC am 08:50 **Enhancing the Analytical Capabilities of DESI Imaging using Ion Mobility Separation- Providing Superior Insights of Biological Samples**; **Emmanuelle Claude**<sup>1</sup>; Emrys A Jones<sup>1,3</sup>; Mark Towers<sup>1</sup>; Karolina Skraskova<sup>2</sup>; Ron M.A. Heeren<sup>2</sup>; Jim Langridge<sup>1</sup>; <sup>1</sup>Waters Corporation, Wilmslow, UK; <sup>2</sup>Maastricht University, Maastricht, NL; <sup>3</sup>Imperial College London, London, UK

TOC am 09:10 **Best of Both Worlds? - Matrix-enhanced SIMS Reveals New Information in Cerebellum Grey and White Matter**; Masoumeh Dowlatshahi Pour<sup>1</sup>; **Per Malmberg**<sup>1</sup>; Andrew Ewing<sup>1,2</sup>; <sup>1</sup>Chalmers University of Technology, Gothenburg, Sweden; <sup>2</sup>University of Gothenburg, Gothenburg, Sweden

TOC am 09:30 **Transmission Geometry MALDI: Assessing Ion Generation/Collection Efficiency at Laser Spot Sizes Down to 1 µm**; **Andre Zavalin**; Junhai Yang; Richard Caprioli; <sup>1</sup>Vanderbilt University, Nashville, TN

TOC am 09:50 **MALDI-2: Sensitive MS Imaging with Laser-Induced Postionization at 5 micrometer pixel size**; **Jens Soltwisch**<sup>1</sup>; Hans Kettling<sup>1,2</sup>; Simeon Vens-Cappell<sup>1,2</sup>; Marcel Wiegelmann<sup>1</sup>; Johannes Müthing<sup>1</sup>; Klaus Dreisewerd<sup>1,2</sup>; <sup>1</sup>Institute for Hygiene, University of Muenster, Muenster, GERMANY; <sup>2</sup>Interdisciplinary Center for Clinical Research, Muenster, Germany

TOC am 10:10 **High Performance MALDI MS Imaging with a Scanning Laser Beam**; **Jan Preisler**<sup>1,2</sup>; Antonin Bednarik<sup>1,2</sup>; Pavel Kuba<sup>3</sup>; Eugene Moskovets<sup>4</sup>; <sup>1</sup>Chemistry Department, Masaryk University, Brno, Czech Republic; <sup>2</sup>CEITEC, Masaryk University, Brno, Czech Republic; <sup>3</sup>FME, University of Technology, Brno, Czech Republic; <sup>4</sup>MassTech, Inc., Columbia, MD

**8:30 – 10:30 AM, TUESDAY MORNING  
 MEMBRANE PROTEINS**  
**Frank Sobott (University of Antwerp) presiding  
 Room 120/127**

TOD am 08:30 **Structure and Dynamics of a Membrane Protein-Surfactant Assembly Studied by Ion-Mobility Mass Spectrometry and Molecular Dynamics Simulations**; Antoni Borysik; **Antoni Borysik**; <sup>1</sup>King's College London, London, UK

TOD am 08:50 **Probing the Structure & Interactions of Membrane Protein Complexes Using Orbitrap Mass Spectrometry**; **Joseph Gault**<sup>1</sup>; Todd Mize<sup>1</sup>; Eugen Damoc<sup>2</sup>; Mikhail Belov<sup>2</sup>; Alexander Makarov<sup>2</sup>;

Carol V. Robinson<sup>1</sup>; <sup>1</sup>Oxford University, Oxford, UK; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany  
 TOD am 09:10 **Membrane Proteins and Complexes: Using an FTMS to “Shake it Off”**; Iain Campuzano<sup>2</sup>; Huilin Li<sup>1</sup>; Dhanashri Bagal<sup>2</sup>; Paul Schnier<sup>2</sup>; **Joseph A. Loo**<sup>1</sup>; <sup>1</sup>UCLA, Los Angeles, CA; <sup>2</sup>AMGEN, Thousand Oaks, CA

TOD am 09:30 **Lipid Binding Induces Conformational Changes in the Peripheral Membrane Protein PDZK1**; **Jamie A. Moroco**<sup>1</sup>; Thomas E. Wales<sup>1</sup>; Jennifer L. Halford<sup>2</sup>; Nadine Elowe<sup>4</sup>; Olivier Kocher<sup>3</sup>; Monty Krieger<sup>2</sup>; John R. Engen<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Massachusetts Institute of Technology, Cambridge, MA; <sup>3</sup>Harvard Medical School, Boston, MA; <sup>4</sup>Broad Institute, Cambridge, MA

TOD am 09:50 **Using Ion Mobility-Mass Spectrometry to Study the Integral Membrane Protein Translocator Protein (TSPO) and its Therapeutic Ligand Binding Behavior**; **Shuai Niu**<sup>1</sup>; Fei Li<sup>2</sup>; Shelagh Ferguson-Miller<sup>2</sup>; Brandon Ruotolo<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>Michigan State University, East Lansing, MI

TOD am 10:10 **Fast size-exclusion Chromatography Electrospray-Ionization Mass Spectrometry of Integral Membrane Proteins**; **Whitaker Cohn**; Joseph Capri; Chris Ryan; Julian Whitelegge; <sup>1</sup>University of California LA, Los Angeles, CA

**8:30 – 10:30 AM, TUESDAY MORNING  
 LIPIDOMICS: NEW MS TECHNOLOGIES AND APPLICATIONS**  
**David Ford (St. Louis University School of Medicine) presiding  
 Theater**

TOE am 08:30 **High Mass Resolution Lipid Imaging: A New Workflow for Guiding FTICR Analysis with High-Speed MALDI TOF Data**; **Jeffrey Spraggins**<sup>1</sup>; Raf Van De Plas<sup>2</sup>; Nico Verbeeck<sup>3</sup>; Etienne Waelkens<sup>3</sup>; Shannon Cornett<sup>4</sup>; Richard Caprioli<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>Delft University of Technology, Delft, Netherlands; <sup>3</sup>K.U. Leuven, Leuven, Belgium; <sup>4</sup>Bruker Daltonics Inc., Billerica, MA

TOE am 08:50 **Abnormal Biogenic Lipid Signalling In Chronic Pain Elucidated With Multimodal Imaging Mass Spectrometry**; **Jorg Hanrieder**<sup>1</sup>; Jie Su<sup>3</sup>; Lorenz Gerber<sup>2</sup>; Kim Kultima<sup>4</sup>; Camilla Svensson<sup>3</sup>; <sup>1</sup>University of Gothenburg, Mölndal, Sweden; <sup>2</sup>SLU, Umeå, Sweden; <sup>3</sup>Karolinska Institute, Stockholm, Sweden; <sup>4</sup>Uppsala University, Uppsala, Sweden

TOE am 09:10 **Separating Lipid Isomers with LC-IMS-MS Measurements to Understand Their Role in Biochemical Processes**; **Erin S. Baker**; Kristin E. Burnum-Johnson; Jennifer E. Kyle; Xing Zhang; Matthew E. Monroe; Yehia M. Ibrahim; Thomas O. Metz; Richard D. Smith; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA

TOE am 09:30 **Multidimensional Mass Spectrometry-based Shotgun Lipidomics Analysis of Vinyl Ether Diglycerides**; **Kui Yang**; Christopher M. Jenkins; Beverly Dilthey; Richard W. Gross; <sup>1</sup>Washington University, St. Louis, MO

TOE am 09:50 **A Shotgun Lipidomics Approach to Study Non-Alcoholic Fatty Liver Disease (NAFLD)**; **Amani Batarseh**<sup>1</sup>; Harry Glickman<sup>1</sup>; David Peake<sup>3</sup>; Alexander Mazur<sup>2</sup>; Peter Metrakos<sup>1</sup>; Tommy Nilsson<sup>1</sup>; <sup>1</sup>RI-MUHC, Montreal, CA; <sup>2</sup>McGill University, Montreal, CA; <sup>3</sup>Thermo Fisher Scientific, San Jose, USA

TOE am 10:10 **Isotopically-labelled TrEnDi: New Technology to Increase the Sensitivity and Selectivity of MS-Based Lipid Analysis of Complex Biological Samples;** Carlos R. Canez; Karl V. Wasslen; Hyunmin Lee; Samuel W. J. Shields; Jeffrey M. Manthorpe; Jeffrey C. Smith; *Carleton University, Ottawa, Canada*

**8:30 – 10:30 AM, TUESDAY MORNING  
PHOSPHOPROTEOMICS IN DISEASE**

**Jun Qu (State University of New York, Buffalo) presiding  
Room 106**

TOF am 08:30 **Kinome Profiling of Glioblastoma Samples by Mass Spectrometry;** Lennard Dekker<sup>1</sup>; Marcel Stoop<sup>1</sup>; Jan-Willem Jachtenberg<sup>1</sup>; Lona Zeneyedpour<sup>1</sup>; Noor Abdhussain<sup>1</sup>; Jos Joore<sup>2</sup>; Sieger Leenstra<sup>1,3</sup>; Theo Luider<sup>1</sup>; *<sup>1</sup>Erasmus Medical Center, Rotterdam, Netherlands; <sup>2</sup>Pepscope, Utrecht, Netherlands; <sup>3</sup>Elisabeth Medical Hospital, Tilburg, Netherlands*

TOF am 08:50 **Unravelling Signaling Pathways in Niemann-Pick type C Disease by “in-vivo” Phosphoproteomic Analysis of Mouse Cerebellum;** Nicolas Lebesgue<sup>1</sup>; Martin Fitzpatrick<sup>1</sup>; Allie Colaco<sup>2</sup>; Frances Platt<sup>2</sup>; Albert J.R. Heck<sup>1</sup>; Simone Lemeer<sup>1</sup>; *<sup>1</sup>Utrecht University, Utrecht, The Netherlands; <sup>2</sup>Oxford University, Oxford, UK*

TOF am 09:10 **Phosphoproteomic and Proteomic Identification of Oncogenic Pathways in LKB1 Dependent Non-Small Cell Lung Cancer by Two-Dimensional LC-MS/MS;** Nilini Ranbaduge; Joseph Amann; Tadaaki Yamada; Zhen Wang; David Carbone; Vicki Wysocki; *The Ohio State University, Columbus, OH*

TOF am 09:30 **Assessment of Rational Peptide Design for Kinase Activity Assays by Mass Spectrometry;** Marcel Stoop<sup>1</sup>; Jetse Scholma<sup>2</sup>; Maikel Peppelenbosch<sup>1</sup>; Jos Joore<sup>3</sup>; Theo Luider<sup>1</sup>; *<sup>1</sup>ErasmusMC, Netherlands, Rotterdam, Netherlands; <sup>2</sup>University of Twente, Enschede, Netherlands; <sup>3</sup>Pepscope B.V., Utrecht, Netherlands*

TOF am 09:50 **Advanced Ti<sup>4+</sup>-IMAC (phospho)proteomics to Identify Novel Melanoma Companion Drug Targets and Uncover Phosphorylation Dynamics and Pathway Dependence in Senescence Signaling;** Violette Gautier<sup>1,2</sup>; Gianluca Maddalo<sup>1,2</sup>; Erik L. de Graaf<sup>1,2</sup>; Joanna Kaplon<sup>3</sup>; Marjon A. Smit<sup>3</sup>; Kristel Kemper<sup>3</sup>; Daniel S. Peeper<sup>3</sup>; Albert J.R. Heck<sup>1</sup>; A.F. Maarten Altelaar<sup>1</sup>; *<sup>1</sup>Utrecht University, Utrecht, Netherlands; <sup>2</sup>Netherlands Proteomics Center, Utrecht, Netherlands; <sup>3</sup>The Netherlands Cancer Institute, Amsterdam, Netherlands*

TOF am 10:10 **Characterization of Regulatory Protein Phosphorylations in Dynamic Golgi Reassembly by Quantitative Label-Free Phosphoproteomic Analysis;** Hye Kyong Kweon; Shijiao Huang; Yanzhuang Wang; Philip Andrews; *University of Michigan, Ann Arbor, MI*

**8:30 – 10:30 AM, TUESDAY MORNING  
EMERGING ENVIRONMENTAL CONTAMINANTS**

**Susan Richardson (University of South Carolina) presiding  
Ballroom 222/224**

TOG am 08:30 **Unequivocal Identification of Detection-Based Transformation Products in Real-World Environmental Samples using High-Resolution MS and NMR;** Damia Barcelo<sup>1,2</sup>; Bozo Zonja<sup>1</sup>; Sandra Perez<sup>1</sup>; Antonio Delgado<sup>3,4</sup>; *<sup>1</sup>Water and Soil Research Group, IDAEA-CSIC, Barcelona, SPAIN; <sup>2</sup>Catalan Institute of Water Research - ICRA, Girona, SPAIN; <sup>3</sup>University of Barcelona (UB); Faculty of Pharmacy, Barcelona, SPAIN; <sup>4</sup>Res. Unit on BioActive Molecules(RUBAM), IQAC-CSIC, Barcelona, Spain*

TOG am 08:50 **Systematic Suspect Screening and Identification of Sulfa Drug Metabolites in the Aquatic Environment;** Marius Majewsky<sup>1</sup>; Thomas Glauner<sup>2</sup>; Craig Marvin<sup>3</sup>; Harald Horn<sup>1,4</sup>; *<sup>1</sup>Karlsruhe Institute of Technology, Water Chemistry, Karlsruhe, Germany; <sup>2</sup>Agilent Technologies Sales & Services GmbH, Waldbronn, Germany; <sup>3</sup>Agilent Technologies Inc., Wilmington, DE; <sup>4</sup>DVGW Research Laboratories, Karlsruhe, Germany*

TOG am 09:10 **Rapid Tracking of ZnO and CeO<sub>2</sub> Nanoparticles through Drinking Water Treatment by Single Particle ICP-MS;** Ariel Donovan<sup>1,2</sup>; Honglan Shi<sup>1,2</sup>; Yinfa Ma<sup>1</sup>; Craig Adams<sup>2,3</sup>; Chady Stephan<sup>4</sup>; Todd Eichholz<sup>5</sup>; *<sup>1</sup>Missouri S&T, Rolla, MO; <sup>2</sup>CS3M, Rolla, MO; <sup>3</sup>Utah State University, Logan, UT; <sup>4</sup>PerkinElmer, Woodbridge, ON; <sup>5</sup>Missouri Department of Natural Resources, Jefferson City, MO*

TOG am 09:30 **Determination of Urinary Metabolites of Organophosphate Flame Retardants Using Ultra Performance Liquid Chromatography (UPLC) Tandem Mass Spectrometry (MS/MS);** Ivana Kosarac<sup>1</sup>; Cariton Kubwabo<sup>1</sup>; Warren Foster<sup>2</sup>; *<sup>1</sup>Environmental and Radiation Health Sciences Direct, Ottawa, Canada; <sup>2</sup>McMaster University, Department of Obstetrics and, Hamilton, Canada*

TOG am 09:50 **Multi-residue Analyses of 71 Endocrine Disruptors in Indoor Air by Liquid and Gas Chromatography Mass Spectrometry Methods;** Stéphanie Laborie<sup>1</sup>; Elodie Moreau-Guigon<sup>1</sup>; Fabrice Alliot<sup>1</sup>; Annie Desportes<sup>1</sup>; Lucie Oziol<sup>2</sup>; Marc Chevreuil<sup>1</sup>; *<sup>1</sup>EPHE, UMR 7619, Paris, France; <sup>2</sup>Université Paris sud, UMR 8079, Orsay, France*

TOG am 10:10 **Identification of 3,5-Dichloro-4-hydroxybenzene Sulfonic Acid as an Unknown Persistent Pollutant in Wastewater Effluent and Natural Water;** M. Paul Chiarelli; Qian Wang; Matthew Reichert; Marlon Lutz; Daniel Becker; *Loyola University, Chicago, IL*

**8:30 – 10:30 AM, TUESDAY MORNING  
LC-MS APPROACHES TO COMBINE TRANSLATIONAL PK/PD BIOMARKERS WITH SMALL MOLECULE ADME WORKFLOWS**

**Darren Dumlao (Pfizer, Inc.) presiding  
Ballroom 220/221**

TOH am 08:30 **LC-MS Determination of Cyclooxygenase, Lipoygenase Enzymatic Mediating Pathways Biomarkers in Rat Colon Microdialysate During Inflammatory Bowel Disease;** Yunan Wang; Craig Lunte; *Department of Chemistry, University of Kansas, Lawrence, KS*

TOH am 08:50 **Biomarker Identification and Evaluation of Therapeutic Efficacy using in vivo Microdialysis coupled with Mass Spectrometry;** Matthew Buczynski; Cristina Irimia; Luis Natividad; Loren Parsons; *The Scripps Research Institute, La Jolla, CA*

TOH am 09:10 **Exploring Phenotypic Cell Metabolism using a LC-HRAMS Metabolic Flux Infrastructure;** John Meissen<sup>1</sup>; Aditi Jatkar<sup>2</sup>; Emily Miller<sup>1</sup>; Russell Miller<sup>2</sup>; Min Wan<sup>2</sup>; Matt Blatnik<sup>1</sup>; *<sup>1</sup>Pfizer, Groton, CT; <sup>2</sup>Pfizer, Cambridge, MA*

TOH am 09:30 **Considerations for a New Strategy of Successful Metabolomics Workflow with Reduced Effort;** Alla Kloss<sup>1</sup>; Sarah Geller<sup>1</sup>; Kristen Randall<sup>1</sup>; Harvey Lieberman<sup>1</sup>; Aharon Cohen<sup>2</sup>; *<sup>1</sup>AR&D, LGCR, Sanofi, Waltham, MA; <sup>2</sup>Waltham, MA*

TOH am 09:50 **Untargeted Stable Isotope Tracing: Establishing A Novel MS-based Strategy for Discovering Metabolic Fate and Flux;** Qiuying Chen; Steven S. Gross; *Weill Medical College of Cornell, New York, NY*





TOH am 10:10 **Quan-Qual in Real-Life Drug Discovery. What Have We Learned and How Do We Move Ahead?** Anne-Charlotte Dubbelman<sup>1</sup>; Lieve Dillen<sup>2</sup>; Gerhard Gross<sup>2</sup>; Filip Cuyckens<sup>2</sup>; Thomas Hankemeier<sup>1</sup>; Rob J. Vreeken<sup>1,2</sup>; <sup>1</sup>LACDR, Leiden University, Leiden, nl; <sup>2</sup>Janssen Pharmaceutica, Beerse, Be

10:30 AM – 2:30 PM, TUESDAY  
TUESDAY POSTER SESSION  
Poster/Exhibit Hall  
Lunch concessions are open 11:00 am – 2:00 pm

TUESDAY AFTERNOON ORAL SESSIONS

2:30 – 4:30 PM, TUESDAY AFTERNOON  
NEW DEVELOPMENTS IN HIGH RESOLUTION AND MASS ACCURACY  
Carolyn J. Cassady (University of Alabama) presiding  
Hall 5

TOA pm 2:30 **Advances in High Field FT-ICR MS: Ultra-High Resolving Power and Mass Accuracy for Environmental and Biological Research;** Jared B. Shaw; Tzu-Yung Lin; Aleksey V. Tolmachev; Errol W. Robinson; David W. Koppenaal; Ljiljana Pasa-Tolic; Pacific Northwest National Laboratory, Richland, WA

TOA pm 2:50 **21 Tesla FT-ICR Mass Spectrometer: A National Resource for Ultrahigh Resolution Mass Spectrometry;** Christopher L. Hendrickson<sup>1,2</sup>; John P. Quinn<sup>1</sup>; Nathan K. Kaiser<sup>1</sup>; Donald F. Smith<sup>1</sup>; Greg T. Blakney<sup>1</sup>; Tong Chen<sup>2</sup>; Alan G. Marshall<sup>1,2</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>FSU Dept of Chemistry and Biochemistry, Tallahassee, FL

TOA pm 3:10 **The New non-FT Method of Super-High Resolution Mass Spectrometry, Based on Measuring of “Antenna” Ion’s Cyclotron Frequency Time Dependence.;** Eugene Nikolaev<sup>1,2</sup>; Gleb Vladimirov<sup>1,3</sup>; Oleg Kharybin<sup>1</sup>; Igor Popov<sup>1,2</sup>; <sup>1</sup>Institute for Energy Problems of Chemical Physics, Moscow, Russia; <sup>2</sup>Moscow Institute of Physics and Technology, Moscow, Russia; <sup>3</sup>Skolkovo Institute of Technology, Moscow, Russia

TOA pm 3:30 **High Resolution on Both Precursor and Fragment Ions in the MS/MS Spectra of Complex Mixtures by Bidimensional FT-ICR MS;** Fabrice bray<sup>1</sup>; Lionel Chiron<sup>4</sup>; Matthias Witt<sup>3</sup>; Marc-André Delsuc<sup>2</sup>; Christian Rolando<sup>1</sup>; <sup>1</sup>Université Lille 1, Villeneuve d’Ascq, France; <sup>2</sup>IGBMC, Université de Strasbourg, Strasbourg, France; <sup>3</sup>Bruker Daltonik, Bremen, Germany; <sup>4</sup>CASC4DE, Strasbourg, France

TOA pm 3:50 **High Resolution and Accurate Mass (HRAM) Characterization of Multiply Charged Proteins by Newly Developed Ionization Techniques on CE-LSI/MAIV-LTQ-Orbitrap Platform;** Bingming Chen; Xuefei Zhong; Chirstopher Lietz; Lingjun Li; University of Wisconsin-Madison, Madison, WI

TOA pm 4:10 **A Fully Integrated GC Orbitrap System Opens a New Chapter in GC-MS;** Paul Silcock<sup>1</sup>; Cristian Cojocariu<sup>1</sup>; Dominic Roberts<sup>1</sup>; Scott T. Quarmby<sup>2</sup>; G.Brody Guckenberger<sup>2</sup>; Jason S. Cole<sup>2</sup>; John G. Voss<sup>2</sup>; Amelia Peterson<sup>3</sup>; Jan-Peter Hauschild<sup>3</sup>; Oliver Lange<sup>3</sup>; Nicholas Kwicien<sup>4</sup>; Michael S. Westphall<sup>4</sup>; Joshua J. Coon<sup>4</sup>; Alexander Makarov<sup>3</sup>; <sup>1</sup>Thermo Fisher Scientific, Runcorn, United Kingdom; <sup>2</sup>Thermo Fisher Scientific, Austin, TX; <sup>3</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>4</sup>University of Wisconsin, Madison, WI

2:30 – 4:30 PM, TUESDAY AFTERNOON  
DATA INDEPENDENT ACQUISITION: INNOVATIVE METHODS AND APPLICATIONS  
Alexander Leitner (ETH Zurich) presiding  
Room 130/132

TOB pm 2:30 **Evaluate SWATH Quantitation using Local and Extended Libraries;** Xiaomin Song; Jemma Wu; Dana Pascovici; Thiri Zaw; Natasha Care; Mark P. Molloy; Australian Proteome Analysis Facility, Sydney, Australia

TOB pm 2:50 **Intrinsic Ratiometric Filters Enhance Precision in Stable Isotope Data-Independent Acquisition Proteomics;** Jaimeen Majmudar; Brent Martin; University of Michigan, Ann Arbor, MI

TOB pm 3:10 **Multi Laboratory Reproducibility and Performance of SWATH™ Acquisition for Proteomic Analyses;** Christie Hunter<sup>1</sup>; Ben Collins<sup>2</sup>; Yansheng Liu<sup>2</sup>; Stefani Thomas<sup>3</sup>; Dan Chan<sup>3</sup>; Hui Zhang<sup>3</sup>; Samuel Bader<sup>4</sup>; Robert Moritz<sup>4</sup>; Birgit Schilling<sup>5</sup>; Bradford Gibson<sup>5</sup>; Christoph Krisp<sup>6</sup>; Mark Molloy<sup>7</sup>; Guixue Hou<sup>8</sup>; Liang Lin<sup>8</sup>; Siqi Liu<sup>8</sup>; Mio Hirayama<sup>9</sup>; Sumio Ohtsuki<sup>9</sup>; Nathalie Selevsek<sup>10</sup>; Ralph Schlapbach<sup>10</sup>; Shin-Cheng Tzeng<sup>11</sup>; Jason Held<sup>11</sup>; Brett Larsen<sup>12</sup>; Anne-Claude Gingras<sup>12</sup>; Ruedi Aebersold<sup>2</sup>; <sup>1</sup>SCIEX, Redwood City, CA; <sup>2</sup>ETH Zurich, Zurich, Switzerland; <sup>3</sup>Johns Hopkins University, Baltimore, MD; <sup>4</sup>Inst Systems Biology, Seattle, WA; <sup>5</sup>Buck Institute for Research on Aging, Novato, CA; <sup>6</sup>Australian Proteome Analysis Facility, Sydney, Australia; <sup>7</sup>Macquarie University, Sydney, Australia; <sup>8</sup>BGI, Shenzhen, China; <sup>9</sup>Univ Kumamoto, Kumamoto, Japan; <sup>10</sup>FGCZ, Univ Zurich, Zurich, Switzerland; <sup>11</sup>Washington University, St. Louis, MO; <sup>12</sup>LTRI, Toronto, ON

TOB pm 3:30 **Data-independent Acquisition using Q Exactive HF to Improve Detection of Urinary Diagnostic Biomarkers of Systemic Diseases;** Jan Muntel<sup>1</sup>; Yue Xuan<sup>2</sup>; Sebastian Berger<sup>1</sup>; Alex Kentesis<sup>4</sup>; Richard Bachur<sup>3</sup>; Hanno Steen<sup>1</sup>; <sup>1</sup>Harvard Medical School/Children’s Hospital Boston, Boston, MA; <sup>2</sup>ThermoFisherScientific, Bremen, Germany; <sup>3</sup>Boston Children’s Hospital, Boston, MA; <sup>4</sup>Cornell University, New York, NY

TOB pm 3:50 **Quantitative Profiling of Circulating Plasma Microparticle Associated Proteins by DDA and DIA nanoLC-MS2;** Manfred Heller; Natasha Buchs; Sophie Braga Lagache; University of Bern, Bern, Switzerland

TOB pm 4:10 **Identification of Archaeal Biofilm Marker Candidates by SWATH-LC/MS/MS Analysis of Planktonic and Sessile Cultures of Halobacterium salinarum R1;** Christof Lenz<sup>1,2</sup>; Gerald Losensky<sup>3</sup>; Sabrina Froels<sup>3</sup>; Felicitas Pfeifer<sup>3</sup>; Henning Urlaub<sup>1,2</sup>; <sup>1</sup>Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; <sup>2</sup>University Medical Center (UMG), Goettingen, Germany; <sup>3</sup>Technical University of Darmstadt, Darmstadt, Germany

## TUESDAY AFTERNOON ORAL SESSIONS

### 2:30 – 4:30 PM, TUESDAY AFTERNOON ION SPECTROSCOPY Jim Prell (University of Oregon) presiding Room 123/124

- TOC pm 2:30 **Fusion of Spectroscopy and Mass Spectrometry for Structural Identification of Biomolecules;** Vladimir Kopysov<sup>1</sup>; Alexander Makarov<sup>2</sup>; Oleg Boyarkin<sup>1</sup>; <sup>1</sup>Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany
- TOC pm 2:50 **Two-Step Energy Transfer Enables Use of Phenylalanine in Action-EET for Distance Constraint Determination in Gaseous Biomolecules;** Nathan Hendricks; Ryan R. Julian; *University of California, Riverside, Riverside, CA*
- TOC pm 3:10 **Photodissociation Action Spectroscopy of Protonated N-Substituted Aromatics: Vibronic Details from Room Temperature Ions;** Christopher Hansen<sup>1</sup>; Stephen J Blanksby<sup>2</sup>; Adam Trevitt<sup>1</sup>; <sup>1</sup>University of Wollongong, Wollongong, Australia; <sup>2</sup>Queensland University of Technology, Brisbane, Australia
- TOC pm 3:30 **Peptide Fragmentation Mechanisms by Infrared Ion Spectroscopy: Recent Advances and Application to ETD;** Jonathan Martens<sup>1</sup>; Josipa Grzetic<sup>1</sup>; Giel Berden<sup>1</sup>; Jos Oomens<sup>1,2</sup>; <sup>1</sup>FELIX Facility - IMM - Radboud University, Nijmegen, The Netherlands; <sup>2</sup>University of Amsterdam, Amsterdam, The Netherlands
- TOC pm 3:50 **Infrared Spectroscopy of Mobility-Selected H<sup>+</sup>Gly-Pro-Gly-Gly (GPPG);** Michael Kamrath<sup>1</sup>; Antoine Masson<sup>1</sup>; Matthew Glover<sup>2</sup>; David Clemmer<sup>2</sup>; Thomas Rizzo<sup>1</sup>; <sup>1</sup>EPFL, Lausanne, Switzerland; <sup>2</sup>Indiana University, Bloomington, IN
- TOC pm 4:10 **Infrared Multiple Photon Dissociation Action Spectroscopy of Mechanically Interlocked Lasso Peptides.;** Kevin Jeanne Dit Fouque<sup>1</sup>; Helene Lavanant<sup>1</sup>; Severine Zirah<sup>2</sup>; Vincent Steinmetz<sup>3</sup>; Philippe Maitre<sup>3</sup>; Sylvie Rebuffat<sup>2</sup>; Carlos Afonso<sup>1</sup>; <sup>1</sup>University of Rouen, Mont Saint Aignan, France; <sup>2</sup>National Museum of Natural History, Paris, France; <sup>3</sup>Université Paris Sud, Orsay, France

### 2:30 – 4:30 PM, TUESDAY AFTERNOON PROTEOMICS: INFECTIOUS DISEASE Julia Chamot-Rooke (Institut Pasteur) presiding Room 120/127

- TOD pm 2:30 **Identification of Staphylococcus aureus Isolates by Shotgun Spectral Matching;** Dana Ohana; Hans Dalebout; Martha van der Beek; Ed Kuijper; Magnus Palmblad; *Leiden University Medical Centre, Leiden, THE NETHERLANDS*
- TOD pm 2:50 **Accurate Characterization of Difficult to Differentiate Pathogens by Intact Protein ESI-HRMS;** Helene Cardasis<sup>2</sup>; Jason Neil<sup>2</sup>; Ping Yip<sup>2</sup>; Eugen Damoc<sup>4</sup>; Roger Grist<sup>3</sup>; Alexander Cherkassky<sup>2</sup>; James Stephenson<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Raleigh, NC; <sup>2</sup>Thermo Fisher Scientific, Cambridge, MA; <sup>3</sup>Thermo Fisher Scientific, East Grinstead, UK; <sup>4</sup>Thermo Fisher Scientific, Bremen, Germany
- TOD pm 3:10 **Proteomic Analysis of the Secretome upon Helicobacter pylori Infection;** Justine Arrington; Xueqin Wang; Daoguo Zhou; Andy Tao; *Purdue University, West Lafayette, IN*
- TOD pm 3:30 **Profiling of Staphylococcus Aureus Secretomes using Bottom-Up and Top-Down Mass Spectrometry;** Jessica Chapman; Elizabeth Ohneck; Divya Balasubramanian; Kayan Tam; Victor Torres; Beatrix Ueberheide; *NYU School of Medicine, New York, NY*

- TOD pm 3:50 **Baccus – a Novel Way of using Targeted Mass Spectrometry to Estimate Bacterial Load;** Ola Kilsgård; Johan Teleman; Erik Malmström; Johan Malmström; *Lund University, Lund, Sweden*
- TOD pm 4:10 **Integrated omics of Influenza A virus: Correlating Glycan Macro and Micro-Heterogeneity with Virus Evolution and Interactions with Host Immune System.;** Kshitij Khatri<sup>1</sup>; Mitchell R. White<sup>1</sup>; Joshua A. Klein<sup>1</sup>; Nancy Leymarie<sup>1</sup>; David F. Smith<sup>2</sup>; Kevan L. Hartshorn<sup>1</sup>; Joseph Zaia<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA; <sup>2</sup>Emory University School of Medicine, Atlanta, GA

### 2:30 – 4:30 PM, TUESDAY AFTERNOON LIPID AND PROFILING Kari Green (University of Florida) presiding Theater

- TOE pm 2:30 **SFC-MS/MS as a New Tool for Global and Quantitative Lipidomics;** Marie Méjean<sup>1</sup>; Laurent Laboureur<sup>1</sup>; Benoit Colsch<sup>2</sup>; Alain Brunelle<sup>1</sup>; David Touboul<sup>1</sup>; <sup>1</sup>Institut de Chimie des Substances Naturelles, CNRS, Gif sur Yvette, France; <sup>2</sup>CEA de SACLAY, Gif sur Yvette, France
- TOE pm 2:50 **Large Scale Lipid Profiling of a Human Serum Lipidome Using a High Resolution Accurate Mass LC/MS/MS Approach;** Reiko Kiyonami<sup>1</sup>; David A. Peake<sup>1</sup>; Xiaodong Liu<sup>2</sup>; Yingying Huang<sup>1</sup>; <sup>1</sup>ThermoFisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific, Sunnyvale, CA
- TOE pm 3:10 **Breast Cancer Tissue Analysis using Photochemical Derivatization and Tandem Mass Spectrometry;** Leelyn Chong; Xiaoxiao Ma; Yu Xia; Zheng Ouyang; *Purdue University, West Lafayette, IN*
- TOE pm 3:30 **Imaging of Changes in Lipids Profile over Time in Traumatic Brain Injury;** Aurelie Roux<sup>1</sup>; Ludovic Muller<sup>1</sup>; Shelley N Jackson<sup>1</sup>; Brian M Cox<sup>2</sup>; J. Albert Schultz<sup>3</sup>; Amina S. Woods<sup>1</sup>; <sup>1</sup>NIH/NIDA-IRP, Baltimore, MD; <sup>2</sup>Uniformed Services University, Bethesda, MD; <sup>3</sup>Ionwerks, Inc, Houston, TX
- TOE pm 3:50 **Single Cell Nanomanipulation to Identify Heterogeneity of Fatty Acid Profiles within Healthy and Diseased Breast Tissue at the Cancer Forefront;** Jason Hamilton; Mandy Phelps; Guido Verbeck; *University of North Texas, Denton, TX*
- TOE pm 4:10 **Assessment of Function of sPLA<sub>2</sub> and Its Receptor PLA2R and Quantification of Intracellular Uptake and Degradation of SPRL by LC-MS/MS;** Ben Nie<sup>1</sup>; Brian S. Cummings<sup>2</sup>; Robert D. Arnold<sup>1</sup>; <sup>1</sup>Harrison School of Pharmacy, Auburn University, Auburn, AL; <sup>2</sup>Wilson College of Pharmacy, University of Georgia, Athens, GA

### 2:30 – 4:30 PM, TUESDAY AFTERNOON PROTEIN-PROTEIN AND PROTEIN-LIGAND INTERACTIONS H. Ewa Witkowska (UCSF) presiding Room 106

- TOF pm 2:30 **Characterization of Large Transient Protein Complexes using Size Exclusion Chromatography with On-Line Detection by Native ESI-MS;** Khaja Muneeruddin; Honglin Yao; Cedric Bobst; Igor A. Kaltashov; *University of Massachusetts, Amherst, MA*
- TOF pm 2:50 **Drug Candidate Screening for Inhibitors of Protein Self-Aggregation using ESI-IMS-MS;** Alison E Ashcroft; Lydia M Young; Janet C Saunders; Rachel A Mahood; Charlotte H Revill; Richard J Foster; Sheena E Radford; *University of Leeds, Leeds, United Kingdom*



- Tof Pm 3:10 **A Platform for the Untargeted Analysis of Protein Interactions**; Owen Skinner<sup>1</sup>; Luis Do Vale<sup>1</sup>; Rafael Melani<sup>1</sup>; Pierre Havugimana<sup>1</sup>; Mikhail Belov<sup>2</sup>; Stevan Horning<sup>3</sup>; Alexander Makarov<sup>3</sup>; Neil L. Kelleher<sup>1</sup>; Philip Compton<sup>1</sup>; <sup>1</sup>Northwestern University, Evanston, IL; <sup>2</sup>Spectrograph LLC, Kennewick, WA; <sup>3</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- TOF pm 3:30 **Time-Resolved Charge Detection Mass Spectrometry of Hepatitis B Virus Capsid Assembly**; Corinne Lutomski; Elizabeth Pierson; Jason Deer; Adam Zlotnick; Martin Jarrold; *Indiana University, Bloomington, IN*
- TOF pm 3:50 **Protein-Glycolipid Interactions Studied *in vitro* using ESI-MS and Nanodiscs. Insights into the Mechanisms and Energetics of Binding**; Ling Han; Elena Kitova; Jun Li; Hong Lin; John Klassen; *University of Alberta, Edmonton, Canada*
- TOF pm 4:10 **Towards a Comprehensive Strategy for Proteome-Wide Characterization of Small Molecule-Protein Interactions.**; Jason Murphy; Scott Brittain; Daniel Palacios; Edmund Harrington; Jason Thomas; Markus Schirle; *Novartis Institutes for BioMedical Research, Inc., Cambridge, MA*
- 2:30 – 4:30 PM, TUESDAY AFTERNOON ENVIRONMENTAL MS: INSTRUMENTAL CHALLENGES AND SOLUTIONS**  
**Lee Ferguson (Duke University) presiding**  
**Ballroom 222/224**
- TOG pm 2:30 **High Resolution and Tandem Mass Spectrometry Uncovers Chlorination Reaction Pathways for Transformation of Medical Imaging Compounds in Drinking Water Treatment**; Susan Richardson<sup>1</sup>; Cristina Postigo<sup>2</sup>; Christina Joseph<sup>1</sup>; Friedrich Wendel<sup>3</sup>; Christian Luetke Eversloh<sup>3</sup>; Thomas Ternes<sup>3</sup>; Edward Machek<sup>4</sup>; Stephen Duirk<sup>4</sup>; Elizabeth Wagner<sup>5</sup>; Michael Plewa<sup>5</sup>; <sup>1</sup>University of South Carolina, Department of Chemis, Columbia, SC; <sup>2</sup>CSIC, Barcelona, Spain; <sup>3</sup>Federal Institute of Hydrology, Koblenz, Germany; <sup>4</sup>University of Akron, Akron, OH; <sup>5</sup>University of Illinois, Urbana, IL
- TOG pm 2:50 **Discovery, Identification and Investigation of Naturally Occurring Antibiotics in Drinking Water using Differential Ion Mobility and Soft Mass Spectrometry**; Jadwiga Lyczko; Wojciech Gabryelski; *University of Guelph, Guelph, Canada*
- TOG pm 3:10 **Direct On-Line Measurement of PAHs in Complex Aqueous Samples: Condensed Phase Membrane Introduction Mass Spectrometry - Direct Electron Ionization (CP-MIMS-DEI)**; Veronica Termopoli<sup>1</sup>; Giorgio Famigliani<sup>1</sup>; Laura Magrini<sup>1</sup>; Pierangela Palma<sup>1</sup>; Erik Krogh<sup>2,3</sup>; Achille Cappiello<sup>1</sup>; Christopher G. Gill<sup>2,3</sup>; <sup>1</sup>University of Urbino, Urbino, Italy; <sup>2</sup>University of Victoria, Victoria, BC, Canada; <sup>3</sup>Appl. Env. Res. Labs. (AERL), Nanaimo, BC, Canada
- TOG pm 3:30 **Identification of Contaminants In House Dust by Two-Dimensional Gas Chromatography and Liquid Chromatography with Mass Spectrometry and Non-Targeted Data Analytics**; Benjamin Place; Jacolin Murray; *National Institute of Standards and Technology, Gaithersburg, MD*
- TOG pm 3:50 **Coupling Atmospheric Pressure Photoionization with Differential Mobility Analysis – Mass Spectrometry for detection of non-polar environmental analytes within gas-phase samples**; Ross McCulloch; Arturo Álvaro Carballido; *SEADM, Boecillo, Spain*
- TOG pm 4:10 **Chemical Characterization of Organic Contaminants in the Environment near an E-Waste Site in China**; Jonathan Byer<sup>3</sup>; Ed Sverko<sup>1</sup>; Kurunthachalam Kannan<sup>2</sup>; Qian Wu<sup>2</sup>; Joe Binkley<sup>3</sup>; <sup>1</sup>Environment Canada, Burlington, ON; <sup>2</sup>Wadsworth Center, New York State Department of Health, Albany, NY; <sup>3</sup>LECO Corporation, St. Joseph, MI
- 2:30 – 4:30 PM, TUESDAY AFTERNOON IMAGING: PHARMACEUTICALS AND METABOLITES**  
**Steve Castellino (GlaxoSmithKline) presiding**  
**Ballroom 220/221**
- TOH pm 2:30 **High Spatial Resolution MALDI Mass Spectrometry Imaging for the Determination of Therapeutic Compound Distribution in Rodent Intestinal Sections**; Anna Nilsson<sup>1</sup>; Alexandra Peric<sup>2</sup>; Marie Strimfors<sup>2</sup>; Eva Lundborg<sup>2</sup>; Richard Goodwin<sup>3</sup>; Martin A. Hayes<sup>2</sup>; Constanze Hilgendorf<sup>2</sup>; Per E. Andren<sup>1</sup>; <sup>1</sup>Uppsala University, Uppsala, Sweden; <sup>2</sup>AstraZeneca, Molndal, SE; <sup>3</sup>AstraZeneca, Cambridge, UK
- TOH pm 2:50 **Insects and Plants: Metabolite Studies using High-Performance AP-MALDI Mass Spectrometry Imaging**; Bernhard Spengler; Andreas Römpf; Dhaka Bhandari; Saleh Khalil; *Analytical Chemistry, Giessen, Germany*
- TOH pm 3:10 **Induced Interstitial Pulmonary Fibrosis (IPF) Model: Unlabeled Bleomycin Distribution and Early IPF Markers Identification by MALDI Imaging**; David Bonnel<sup>1</sup>; Mary McElroy<sup>2</sup>; Emeline Falaux<sup>1</sup>; Fabien Pamelard<sup>1</sup>; Gael Picard de Muller<sup>1</sup>; Gregory Hamm<sup>1</sup>; Stephen Madden<sup>2</sup>; Jonathan Stauber<sup>1</sup>; <sup>1</sup>ImaBiotech, MS Imaging Dept., Loos, France; <sup>2</sup>Charles River Discovery Research Services, Edinburgh, United-Kingdom
- TOH pm 3:30 **Multiplatform Mass Spectrometry Imaging to Detect and Differentiate Nanoparticle Formulated and Released Drug in Preclinical Tumors**; Richard Goodwin<sup>1</sup>; John Swales<sup>1</sup>; Anna Nilsson<sup>2</sup>; Per E Andren<sup>2</sup>; Nicole Strittmatter<sup>3</sup>; Zoltan Takats<sup>3</sup>; Susan Ashton<sup>4</sup>; Philip Jewsbury<sup>4</sup>; Peter Webb<sup>4</sup>; Simon Barry<sup>4</sup>; <sup>1</sup>AstraZeneca, Cambridge, UK; <sup>2</sup>Uppsala University, Uppsala, SE; <sup>3</sup>Imperial College, London, UK; <sup>4</sup>AstraZeneca, Maccelsfield, UK
- TOH pm 3:50 **The Applications of Single-probe Mass Spectrometry: Single Cell Analysis and Biological Tissue Imaging**; Ning Pan; Wei Rao; Mei Sun; Zhibo Yang; *University of Oklahoma, Norman, OK*
- TOH pm 4:10 **Molecular Imaging of Antibiotic Inhibition of Bacterial Growth and Metabolism by Laser Ablation Electrospray Ionization Mass Spectrometry**; Pranav Balan<sup>1</sup>; Hang Li<sup>2</sup>; Akos Vertes<sup>2</sup>; <sup>1</sup>Thomas Jefferson HS for Science and Technology, Alexandria, VA; <sup>2</sup>George Washington University, Washington, DC

## TUESDAY AFTERNOON AND WEDNESDAY MORNING ORAL SESSIONS

### 4:45 – 5:30 PM, TUESDAY AFTERNOON AWARD LECTURE

Jenny Brodbelt (University of Texas, Austin) presiding  
Hall 5

Presentation of the 2015 Research Awards



**Biemann Medal**

**Michael J. MacCoss**  
University of Washington

### 5:45 – 7:00 PM, TUESDAY AFTERNOON WORKSHOPS

There are light refreshments in the common areas.

01. Laboratory Developed Test Guidance and Mass Spectrometric Diagnostics: Impact and Expectations, Room 130
02. Current Trends, Gaps, and Needs in Workflows for Targeted Protein Quantitation by LC/MS, Room 131
03. ProeomicsDB, Room 132

04. FTMS: MS/MS at High Resolution, Room 123/124
05. Identifying Tandem Mass Spectra of Lipids and Carbohydrates, Room 120/127
06. MS Analysis of Antibody-Drug Conjugates, Room 260/267
07. Measuring the exposome: Strategies and preliminary results, Room 274
08. Advancements and Discussion of Mass Spectrometry Technology and Challenges within the Polymer and Material Fields, Room 275
09. The ABCs of Being a Great Reviewer for Scientific Journals, Room 230
10. How to Network without Really Trying: A Forum for Current (and Future) Mass Spectrometrists in Industry, Room 231
11. Room 232
12. Invalidating your Cores Data: Examples on How to Check your Data and Report Results and Communicate Invalid or Bad Results to your Customers, Ballroom 222/224
13. How Can Ion Mobility Spectrometry Separations Help your research? Ballroom 220/221

**AFTER 8:00 PM  
CORPORATE HOSPITALITY SUITES  
RENAISSANCE GRAND HOTEL**

## WEDNESDAY MORNING ORAL SESSIONS

### 8:30 – 10:30 AM, WEDNESDAY MORNING AMBIENT AND ATMOSPHERIC PRESSURE GENERATION OF MULTIPLY-CHARGED IONIC SPECIES

Abraham Badu-Tawiah (Ohio State University) presiding  
Hall 5

- WOA am 08:30 **How are Nearly Identical Charge States Produced from the Solution (ESI) and Solid (MAIV) States;** Charles N. McEwen<sup>1,2</sup>; Sarah Trimpin<sup>3,4</sup>; <sup>1</sup>Univ. of the Sciences, Philadelphia, PA; <sup>2</sup>MSTM, Newark, Delaware; <sup>3</sup>Cardiovascular Research Center, WSU, Detroit, MI; <sup>4</sup>Wayne State University, Detroit, MI
- WOA am 08:50 **A Suite of Liquid UV-AP-MALDI Techniques for the Generation of Multiply Charged Ions at High Sensitivity with Stable, Long-Lasting Yield;** Pavel Ryumin<sup>1</sup>; Jeff Brown<sup>1,2</sup>; Mike Morris<sup>2</sup>; Rainer Cramer<sup>1</sup>; <sup>1</sup>University of Reading, Reading, UK; <sup>2</sup>Waters Corporation, Wilmslow, UK
- WOA am 09:10 **Improving the Analysis of Proteins by Desorption Electrospray Ionization (DESI) by the Addition of Ammonium Bicarbonate;** Andre Venter; Elahe Honarvar; Western Michigan University, Kalamazoo, MI
- WOA am 09:30 **Effects of Supercharging Reagents on Protein Stability in Bulk Solution and Insight into the Mechanism of Supercharging;** Catherine Going; Beryl Xia; Evan Williams; Berkeley, CA
- WOA am 09:50 **Molecular Dynamics Simulations Yield Atomistic Insights Into Electropray Mechanisms: From Salt Clusters to Protein Ions;** Lars Konermann; Robert G. McAllister; Haidy Metwally; Univ. of Western Ontario, London, Canada
- WOA am 10:10 **Particle Size Selected Inlet Ionization;** Kermit K. Murray; Fan Cao; Fabrizio Donnarumma; Louisiana State University, Baton Rouge, LA

### 8:30 – 10:30 AM, WEDNESDAY MORNING INFORMATICS: PRM AND DIA

Brendan MacLean (University of Washington) presiding  
Room 130/132

- WOB am 08:30 **Targeted Analysis of MS1 Only DIA Data;** Oliver M. Bernhardt<sup>1</sup>; Roland M. Bruderer<sup>1</sup>; Yue Xuan<sup>2</sup>; Tejas Gandhi<sup>1</sup>; Paul Boersema<sup>3</sup>; Paola Picotti<sup>3</sup>; Lukas Reiter<sup>1</sup>; <sup>1</sup>Biognosys AG, Zuerich, Switzerland; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>3</sup>Institute of Biochemistry, ETH, Zuerich, Switzerland
- WOB am 08:50 **Using DIA to Predict High-Responding Peptides for Targeted Proteomics Experiments;** Brian C. Searle<sup>1,2</sup>; Jarrett D. Egertson<sup>1</sup>; James G. Bollinger<sup>1</sup>; Michael J. MacCoss<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Proteome Software Inc., Portland, OR
- WOB am 09:10 **Making the Transition from Targeted to DIA: Genetic Algorithms Enable Assay Portability;** Jacob D. Jaffe; Jennifer Abelin; Steven A. Carr; The Broad Institute, Cambridge, MA
- WOB am 09:30 **Towards a "Load and Play" Solution for Parallel Reaction Monitoring Assays;** Bruno Doman; Sang Yoon Kim; Daniel Ayoub; Sebastien Gallien; Luxembourg Clinical Proteomics Center, Strassen, Luxembourg
- WOB am 09:50 **Sensitive Peptide Identification in Data-Independent Acquisition by Spectral Library Search;** Jian Wang<sup>1</sup>; Monica Tucholska<sup>2</sup>; Brett Larsen<sup>2</sup>; Anne-Claude Gingras<sup>2</sup>; Nuno Bandeira<sup>3</sup>; <sup>1</sup>UCSD, La Jolla, CA; <sup>2</sup>Lunenfeld-Tanenbaum Research Institute, Toronto, Canada; <sup>3</sup>University of California, San Diego, La Jolla, CA
- WOB am 10:10 **Toward an Optimal Computational Strategy for DIA Mass Spectrometry Data;** Chih-Chiang Tsou<sup>1</sup>; Anne-Claude Gingras<sup>2</sup>; Alexey Nesvizhskij<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>Samuel Lunenfeld Research Institute, Mount Sinai H, Toronto, ON



8:30 – 10:30 AM, WEDNESDAY MORNING  
ION MOBILITY: STRUCTURES

Kevin Giles (Waters Corporation) presiding  
Room 123/124

- WOC am 08:30 **Mobility Calculations from Small Ions to Macromolecular Complexes using the Electronic Surface Representation**; Yuri Alexeev<sup>1</sup>; Joseph Insley<sup>1</sup>; Dmitri Fedorov<sup>2</sup>; Alexandre Shvartsburg<sup>3</sup>; <sup>1</sup>Argonne National Laboratory, Argonne, IL; <sup>2</sup>Nanosystem Research Institute, Tsukuba, Japan; <sup>3</sup>Wichita State University, Wichita, KS
- WOC am 08:50 **Pushing the Boundaries of Small Molecule Analysis: using Ion Mobility MS and Gas-Phase Infrared Spectroscopy To Study Protonation Site Isomers**; Jasper Boschmans<sup>1</sup>; Stephan Warnke<sup>2</sup>; Jongcheol Seo<sup>2</sup>; Jonathan P. Williams<sup>3</sup>; Kevin Pagel<sup>2,4</sup>; Gert von Helden<sup>2</sup>; Filip Lemière<sup>1</sup>; Frank Sobott<sup>1</sup>; <sup>1</sup>University of Antwerp, Antwerp, Belgium; <sup>2</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany; <sup>3</sup>Waters Corporation, Manchester, UK; <sup>4</sup>Freie Universität Berlin, Berlin, Germany
- WOC am 09:10 **Ion Mobility-Mass Spectrometry Reveals the Energy Landscape of Polyproline Folding**; Liuqing Shi<sup>1</sup>; Alison Holliday<sup>2</sup>; Matthew Glover<sup>1</sup>; Michael Ewing<sup>1</sup>; David Russell<sup>3</sup>; David Clemmer<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN; <sup>2</sup>Moravian College, Bethlehem, PA; <sup>3</sup>Texas A&M University, College Station, TX
- WOC am 09:30 **Structural Analysis of Monomeric and Dimeric Neuropeptide Y (NPY) with IM-MS, HDX MS, and MD simulations**; Xueqin Pang<sup>1</sup>; Christopher B. Lietz<sup>2</sup>; Lingjun Li<sup>1</sup>; <sup>1</sup>School of Pharmacy, University of Wisconsin, Madison, WI; <sup>2</sup>Department of Chemistry, University of Wisconsin, Madison, WI
- WOC am 09:50 **HDX-TIMS-MS and Molecular Dynamics Reveal Folding Pathways in DNA-Binding Proteins**; Emily Schenk<sup>1</sup>; Frederic Nau<sup>1</sup>; Genevieve Gozo<sup>1</sup>; Mark Ridgeway<sup>2</sup>; Melvin A. Park<sup>3</sup>; Fenfei Leng<sup>1</sup>; Francisco Fernandez Lima<sup>1</sup>; <sup>1</sup>Florida International University, Miami, FL; <sup>2</sup>Bruker Daltonics, Billerica, MA; <sup>3</sup>Bruker Daltonics, Inc., Billerica, MA
- WOC am 10:10 **Novel Insights into the Structural Dynamics and Effects of Ligand-Binding on Protein Kinase A using Ion Mobility-Mass Spectrometry**; Matthias Vonderach; Dominic Byrne; Samantha Ferries; Patrick Eyers; Claire Eyers; University of Liverpool, Liverpool, UK

8:30 – 10:30 AM, WEDNESDAY MORNING  
CARBOHYDRATES

Robert Chalkley (UCSF) presiding  
Room 120/127

- WOD am 08:30 **Characterization of Highly Heterogeneous Protein-Heparin Complexes using Novel Mass Spectrometry-Based Approaches**; Yunlong Zhao; Rinat Abzalimov; Igor A. Kaltashov; University of Massachusetts, Amherst, MA
- WOD am 08:50 **A New Image of Wheat Cell Walls Revealed through MS Imaging and Ion Mobility**; Dušan Veličković; Fabienne Guillon; Luc Saulnier; Hélène Rogniaux; INRA, Nantes, France
- WOD am 09:10 **Resin-Based and Magnetic Nanoparticle-Based Biomimetic Reagents for Glycan Structure Determination by Mass Spectrometry**; Jinshan Gao; Jungeun Lee; Nikunj Desai; Montclair State University, Montclair, NJ
- WOD am 09:30 **Coupling of FANGS to the INLIGHT™ Strategy for Accurate Relative Quantification of N-Glycans Derived from Minimal Biological Material**; Elizabeth S. Hecht; James P. McCord; Rebecca

Wysocky; James N. Petite; David C. Muddiman; North Carolina State University, Raleigh, NC

- WOD am 09:50 **The Use of Isotopically Labeled IgG for the Relative and Absolute Quantitation of N-linked Glycans**; Ron Orlando<sup>1,2</sup>; Shujuan Tao<sup>1</sup>; Yining Huang<sup>1</sup>; Emily Betchy<sup>1</sup>; Barry Boyes<sup>2,3</sup>; Alex Harvey<sup>2</sup>; <sup>1</sup>Complex Carbohydrate Research Center, UGA, Athens, GA; <sup>2</sup>GlycoScientific, LLC, Athens, GA; <sup>3</sup>Advanced Materials Technology Inc., Wilmington, DE
- WOD am 10:10 **Integrated Glycomics and Proteomics Study for Astrocytoma from 118 Patient Samples**; Chun Shao; Lilla Turiak; Nancy Leymarie; Joseph Zaia; Boston University School of Medicine, Boston, MA

8:30 – 10:30 AM, WEDNESDAY MORNING  
FT, ION TRAPS AND HYBRID INSTRUMENTS  
Eugene Nikolaev (Institute for Energy Problems and Chemical Physics) presiding  
Theater

- WOE am 08:30 **Experimental Investigation of Linear Quadrupole and Octopole Ion Traps for External Ion Accumulation for High Field FT-ICR MS**; Donald F. Smith<sup>1</sup>; Nathan K. Kaiser<sup>1</sup>; John P. Quinn<sup>1</sup>; Steven C. Beu<sup>2</sup>; Alan G. Marshall<sup>1,3</sup>; Christopher L. Hendrickson<sup>1</sup>; <sup>1</sup>National High Magnetic Field Laboratory, FSU, Tallahassee, FL; <sup>2</sup>S C Beu Consulting, Austin, TX; <sup>3</sup>Dept. Chem. & Biochem., Florida State University, Tallahassee, FL
- WOE am 08:50 **Towards Parallel Mass Spectrometry with a Novel Multi-Quadrupole Ion Trap (MultiQ-IT)**; Andrew N. Krutchinsky; Herbert Cohen; Brian T. Chait; The Rockefeller University, New York, NY
- WOE am 09:10 **Time-Dependent Modulation of Reflectron Plate Potential for Increased Charge Density and Reduced Dephasing in an Electrostatic Linear Ion Trap**; Eric Dziekonski; Scott McLuckey; Purdue University, West Lafayette, IN
- WOE am 09:30 **Middle Down Proteomics by MS3 on a Tribrid Mass Spectrometer**; Jolene K. Diedrich; Mathieu Lavallée-Adam; Antonio F. M. Pinto; James J. Moresco; John R. Yates III; The Scripps Research Institute, La Jolla, CA
- WOE am 09:50 **Parallel Detection of Ions with an ICR Cell Array**; Sung-Gun Park<sup>1</sup>; Gordon Anderson<sup>2</sup>; James Bruce<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>GAA Custom Engineering, LLC, Benton, WA
- WOE am 10:10 **Novel mass analyzers for rapid high-performance FT-ICR MS**; Yury Tsybin<sup>1,2</sup>; Anton Kozhinov<sup>1</sup>; Konstantin Nagornov<sup>1</sup>; <sup>1</sup>Ecole Polytechnique Federale, Lausanne, Switzerland; <sup>2</sup>Spectroswiss Sàrl, Lausanne, Switzerland

8:30 – 10:30 AM, WEDNESDAY MORNING  
MASS SPECTROMETRY IN STRUCTURAL BIOLOGY  
Arthur Laganowsky (Texas A&M Health Science) presiding  
Room 106

- WOF am 08:30 **Measuring the Binding Interfaces of Protein Complexes by Gas-Phase Hydrogen/Deuterium Exchange Mass Spectrometry (Gas-Phase HDX-MS)**; Ulrik H. Mistarz<sup>1</sup>; Jeffery M. Brown<sup>2</sup>; Kim F. Haselmann<sup>3</sup>; Kasper D. Rand<sup>1</sup>; <sup>1</sup>Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; <sup>2</sup>Waters MS Technologies Centre, Wilmslow, U. K.; <sup>3</sup>Diabetes Protein Engineering, Novo Nordisk A/S, Måløv, Denmark

WOF am 08:50 **Development of Isotope-Encoded Protein Footprinting for Mass Spectrometry-based Protein Conformational Studies;** Hao Zhang; Haijun Liu; Michael L. Gross; Robert E. Blankenship; *Washington University, Saint Louis, MO*

WOF am 09:10 **Distinctive Structural Dynamics in Ras and Related Proteins by Hydrogen Exchange Mass Spectrometry;** Rane Harrison<sup>1</sup>; Martin Carrasco<sup>2</sup>; John Hunter<sup>2</sup>; Anuj Manandhar<sup>2</sup>; Kenneth Westover<sup>2</sup>; John Engen<sup>1</sup>; <sup>1</sup>*Northeastern University, Boston, MA*; <sup>2</sup>*University of Texas Southwestern Medical Center, Dallas, TX*

WOF am 09:30 **Mass Spectrometry for Monitoring the Transfer of Iron-Sulfur Clusters between Proteins;** William K. Russell; James Vranish; David Barondeau; David Russell; *Texas A&M University, College Station, TX*

WOF am 09:50 **Structure Elucidation of Toyocamycin Nitrite Hydratase, a Hetero-hexameric Protein Complex, by Mass Spectrometry;** Yang Song<sup>1</sup>; Micah Nelp<sup>2</sup>; Vahe Bandarian<sup>2</sup>; Vicki H. Wysocki<sup>1</sup>; <sup>1</sup>*The Ohio State University, Columbus, OH*; <sup>2</sup>*The University of Arizona, Tucson, AZ*

WOF am 10:10 **Using Cross-Linking Coupled to Mass Spectrometry and Integrated Modeling to Study the Molecular Architecture of Large Protein Assemblies;** Florian Stengel<sup>1,2</sup>; Erzberger Jan<sup>1</sup>; Riccardo Pellarin<sup>3</sup>; Suyang Zhang<sup>1</sup>; Tanja Schaefer<sup>1</sup>; Christopher H. S. Aylett<sup>1</sup>; Peter Cimermančič<sup>3</sup>; Daniel Boehringer<sup>1</sup>; Andrej Sali<sup>3</sup>; Ruedi Aebersold<sup>1</sup>; Nenad Ban<sup>1</sup>; <sup>1</sup>*ETH Zurich, Zurich, Switzerland*; <sup>2</sup>*University of Konstanz, Konstanz, Germany*; <sup>3</sup>*University of California, San Francisco, CA*

**8:30 – 10:30 AM, WEDNESDAY MORNING  
EPIGENETIC MODIFICATIONS AND MECHANISMS  
Kangling Zhang (University of Texas, Galveston) presiding  
Ballroom 222/224**

WOG am 08:30 **Modifications of the Mind: RNA Modifications Profile of Differentiated Human Frontal Cortex Cells;** Maria Basanta-Sanchez<sup>1</sup>; Subhrakanti Saha<sup>1</sup>; Sally Temple<sup>2</sup>; Mo Liu<sup>2</sup>; Paul Agris<sup>1</sup>; <sup>1</sup>*The RNA Institute, University at Albany, Albany, NY*; <sup>2</sup>*Neural Stem Cell Institute, Rensselaer, NY*

WOG am 08:50 **Towards Understanding the Dynamics of Histone Combinatorial Proteoforms using a Boosted Middle-Down Proteomics Platform;** Simone Sidoli<sup>1</sup>; Chrystian Ruminowicz<sup>2</sup>; Kelly Karch<sup>1</sup>; Shu Lin<sup>1</sup>; Benjamin A. Garcia<sup>1</sup>; <sup>1</sup>*University of Pennsylvania, Philadelphia, PA*; <sup>2</sup>*Private developer, Białystok, Poland*

WOG am 09:10 **Analysis of Histone Posttranslational Modifications on Nascent Chromatin;** Constance Alabert<sup>1</sup>; Teresa Barth<sup>2</sup>; Axel Imhof<sup>2</sup>; Anja Groth<sup>1</sup>; <sup>1</sup>*Biotech Research and Innovation Centre (BRIC), Copenhagen, Denmark*; <sup>2</sup>*Adolf-Butenandt-Institute, Munich, Germany*

WOG am 09:30 **A Top-Down Approach to Decoding Histones Using a Modified Tribid Mass Spectrometer with Improved Vacuum and ETD Performance;** Yupeng Zheng<sup>1</sup>; Luca Fornelli<sup>1</sup>; Philip D. Compton<sup>1</sup>; Seema Sharma<sup>2</sup>; Jesse D. Canterbury<sup>2</sup>; Christopher Mullen<sup>2</sup>; Vlad Zabrouskov<sup>2</sup>; Jon A. Oyer<sup>1</sup>; Jonathan D. Licht<sup>1</sup>; Michael W. Senko<sup>2</sup>; Neil L. Kelleher<sup>1</sup>; <sup>1</sup>*Northwestern University, Evanston, IL*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*

WOG am 09:50 **Unraveling Site-Specific Acetylation using High Resolution Mass Spectrometry in HATs and HDACs Mutants of Fission Yeast;** Nebiyu Abshiru<sup>1,2</sup>; Roshan Rajan<sup>1,2</sup>; Alain Verreault<sup>1,2</sup>; Pierre Thibault<sup>1,2</sup>; <sup>1</sup>*University of Montreal, Montreal, QC, Canada*; <sup>2</sup>*Institute for Research in Immunology and Cancer, Montreal, QC, Canada*

WOG am 10:10 **Mass Spectrometry-Based Characterization of Histone Methylation in Microglia after Ethanol Exposure;** Joao Paulo Costa Pinho<sup>1</sup>; Jennifer Guergues<sup>1</sup>; Harris Bell-Temin<sup>1</sup>; Bin Liu<sup>2</sup>; Stanley M. Stevens, Jr.<sup>1</sup>; <sup>1</sup>*University of South Florida, Tampa, FL*; <sup>2</sup>*University of Florida, Gainesville, FL*

**8:30 – 10:30 AM, WEDNESDAY MORNING  
APPLICATION OF STABLE ISOTOPE LABELING IN MS ANALYSIS  
OF SMALL MOLECULES AND PROTEINS  
Mingshe Zhu (Bristol-Myers Squibb) presiding  
Ballroom 220/221**

WOH am 08:30 **LC-MS Methods to Profile the Cow Milk Metabolome and Determine the Effects of Milk Consumption on the Human Urine Metabolome;** Dorothea Mung; Liang Li; *University of Alberta, Edmonton, Canada*

WOH am 08:50 **Developmental Stage of Tomato Leaves Determines the Diversity and Dynamics of Trichome Specialized Metabolites;** Zhenzhen Wang; A. Daniel Jones; *Michigan State University, East Lansing, MI*

WOH am 09:10 **Platelet Biomarkers of Metabolic Disturbances in Friedreich's Ataxia;** Andrew J. Worth<sup>1</sup>; Sankha S. Basu<sup>2</sup>; Eric C. Deutsch<sup>3</sup>; Wei-Ting Hwang<sup>1</sup>; Nathaniel W Snyder<sup>1</sup>; David R. Lynch<sup>3</sup>; Ian A. Blair<sup>1</sup>; <sup>1</sup>*University of Pennsylvania, Philadelphia, PA*; <sup>2</sup>*Brigham & Women's Hospital, Harvard, Boston, MA*; <sup>3</sup>*Departments of Neurology and Pediatrics, CHOP, Philadelphia, PA*

WOH am 09:30 **Hyperplex Amino Acid-based Isobaric Labels for Quantitative Proteomics;** Qing Yu<sup>1</sup>; Tyler Greer<sup>2</sup>; Lingjun Li<sup>3</sup>; <sup>1</sup>*University of Wisconsin-Madison, Madison, Wisconsin*; <sup>2</sup>*University of Wisconsin-Madison, Middleton, WI*; <sup>3</sup>*University of Wisconsin, Madison, WI*

WOH am 09:50 **A Novel Triplex Isobaric Peptide Termini Labeling Approach for Quantitative Proteomics;** Haojie Lu; Hongrui Yin; Lei Zhang; Liqi Xie; Ying Zhang; *Fudan University, Shanghai, CHINA*

WOH am 10:10 **Large Scale Metabolic Exploration of Human CSF Proteins using Stable Isotope Labeling Amino Acid *in-vivo* (SILAV);** Sylvain Lehmann<sup>1</sup>; Jérôme Vialaret<sup>1</sup>; Guillaume Gras Combe<sup>2</sup>; Luc Bauchet<sup>2</sup>; Mamadou Lamine Tall<sup>3</sup>; Olivier Hanon<sup>4</sup>; Audrey Gabelle<sup>5</sup>; Christophe Hirtz<sup>1</sup>; <sup>1</sup>*CHRU de Montpellier and Université de Montpellier, Montpellier, France*; <sup>2</sup>*Service de Neurochirurgie, CHRU de Montpellier, Montpellier, France*; <sup>3</sup>*Pharmacie, Groupement Hospitalier Edouard Herriot, Lyon, France*; <sup>4</sup>*AP-HP, Hôpital Broca, Service de Gériatrie, Paris, France*; <sup>5</sup>*Centre Mémoire Ressources CHRU Montpellier, Montpellier, France*

**10:30 AM – 2:30 PM, WEDNESDAY  
WEDNESDAY POSTER SESSION  
Poster/Exhibit Hall  
Lunch concessions are open 11:00 am – 2:00 pm**



**2:30 – 4:30 PM, WEDNESDAY AFTERNOON  
AMBIENT IONIZATION: INSTRUMENTATION AND APPLICATIONS**  
Douglas F. Barofsky (Oregon State University) presiding  
Hall 5

- WOA pm 2:30 **Development of a New Versatile Instrument Combining Laser Ablation Mass Spectrometry and Laser Emission Spectroscopy;** Andreas Bierstedt<sup>1</sup>; Ulrich Panne<sup>1,2</sup>; Jens Riedel<sup>1</sup>; <sup>1</sup>BAM Federal Institute for Materials, Berlin, Germany; <sup>2</sup>Humboldt University, Berlin, Germany
- WOA pm 2:50 **Species Identification by Chemotaxonomy, Ambient Ionization, and Chemometrics with Hierarchical Clustering.;** Rabi Musah<sup>2</sup>; Robert B. Cody<sup>1</sup>; Edgard Espinoza<sup>3</sup>; Ashton Lesiak<sup>4</sup>; Earl Christensen<sup>5</sup>; Hannah Moore<sup>6</sup>; Simin D. Maleknia<sup>7</sup>; <sup>1</sup>JEOL USA, Inc., Peabody, MA; <sup>2</sup>University at Albany-SUNY, Albany, NY; <sup>3</sup>US National Fish and Wildlife Forensics Laboratory, Ashland, OR; <sup>4</sup>University at Albany, Albany, New York; <sup>5</sup>National Renewable Energy Laboratory, Golden, CO; <sup>6</sup>Keele University, Keele, UK; <sup>7</sup>University of New South Wales, Sydney, Australia
- WOA pm 3:10 **Development of a Solid-Phase Micro Extraction-Dielectric Barrier Discharge Ionization-Mass Spectrometry (SPME-DBDI-MS) Direct Coupling under Ambient Conditions: Approaching ppq Sensitivity;** Mario Francesco Mirabelli; Jan-Christoph Wolf; Renato Zenobi; *ETH Zurich, Switzerland, CH*
- WOA pm 3:30 **Rapid Discrimination of Human Skin-related Microorganisms *in vitro* by Ambient Ionization Mass Spectrometry;** Pu Wei<sup>1</sup>; Alan Jamusch<sup>1</sup>; Ahmed M. Hamid<sup>1</sup>; Valentina Pirro<sup>1</sup>; Rafal M. Pielak<sup>2</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>L'Oréal California Research Center, San Francisco, CA
- WOA pm 3:50 **Coupling Charge Reduction Mass Spectrometry to Liquid Chromatography for Complex Mixture Analysis;** John Stutzman; Matthew Crowe; James Alexander IV; Bruce Bell; *The Dow Chemical Company, Collegetown, PA*
- WOA pm 4:10 **Demonstrating the use of Surface Acoustic Wave Nebulization (SAWN) on Multiplex Assay of Lysosomal Storage Diseases;** Angelo Condulle; Frantisek Turecek; *University of Washington, Seattle, WA*

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON  
INFORMATICS: PROTEIN IDENTIFICATION AND QUANTIFICATION**  
Oliver Kohlbacher (Universitat Tübingen) presiding  
Room 130/132

- WOB pm 2:30 **Top-Down Proteogenomics;** Mikhail Kolmogorov; Pavel Pevzner; *UCSD, La Jolla, CA*
- WOB pm 2:50 **MSPathFinder: An Open Source Proteoform Identification and Quantification Tool for Top-Down Proteomics;** Sangtae Kim; Christopher S. Wilkins; Jungkap Park; Paul D. Piehowski; Anil K. Shukla; Yufeng Shen; Samuel H. Payne; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- WOB pm 3:10 **Picked Protein FDR, a Scalable Approach for Protein False Discovery Rate Estimation in Large Proteomic Data Sets;** Mathias Wilhelm<sup>1</sup>; Mikhail Savitski<sup>2</sup>; Hannes Hahne<sup>1</sup>; Bernhard Kuster<sup>1</sup>; Marcus Bantscheff<sup>2</sup>; <sup>1</sup>Technische Universität München, Freising, Germany; <sup>2</sup>Cellzome GmbH a GSK company, Heidelberg, Germany

- WOB pm 3:30 **Protein Identification with Accurate Statistical Significance Assignment using Mass Spectrometry;** Gelio Alves; Aleksey Ogurtsov; Yi-Kuo Yu; *National Center for Biotechnology Information, NLM, Bethesda, MD*
- WOB pm 3:50 **Controlling False Discovery Rates (FDRs) in Genome-Wide Proteomics Datasets;** Stefka Tyanova; Pavel Sinitcyn; Matthias Mann; Juergen Cox; *Max-Planck-Institute of Biochemistry, Martinsried, GERMANY*
- WOB pm 4:10 **“How to Recover from a Bad Day” Data Processing Tolerant to Experimental Errors;** Amandine Boudreau; Gordana Ivosev; Vlad Savchenko; CJ Baker; Suyu Liu; Stephen A Tate; *Sciex, Concord, Canada*

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON  
REACTIONS, DYNAMICS AND THEORY OF GAS PHASE IONS**  
Zhibo Yang (University of Oklahoma) presiding  
Room 123/124

- WOC pm 2:30 **Does Spin-Orbit Coupling Really Matter? The Interesting Case of Th<sup>+</sup> + CH<sub>4</sub>;** Peter Armentrout<sup>1</sup>; Richard M. Cox<sup>1</sup>; Wibe de Jong<sup>2</sup>; <sup>1</sup>University of Utah, Salt Lake City, UT; <sup>2</sup>Lawrence Berkeley National Laboratory, Berkeley, CA
- WOC pm 2:50 **Binding of Xe and Perfluorinated Compounds Inside Cucurbit[n]uril Hosts: Computational and Experimental Results and Anomalous Dissociation;** Conner Harper; David V. Dearden; *Brigham Young University, Provo, UT*
- WOC pm 3:10 **Opposing Charges in ESI-MS of Noncovalent Complexes Explain Many Observations;** Rachel Loo; Huilin Li; Joseph A. Loo; *UCLA, Los Angeles, CA*
- WOC pm 3:30 **Using MS to Invent a New Metal Catalyzed “Molecular Switcheroo” Reaction;** Richard A. J. O’hair<sup>1</sup>; George N. Khairallah<sup>2</sup>; Jiawei Li<sup>1</sup>; Paul Donnelly<sup>1</sup>; Asif Noor<sup>2</sup>; <sup>1</sup>University of Melbourne, Victoria, AUSTRALIA; <sup>2</sup>Bio21 Inst, Uni of Melbourne, Melbourne, AUSTRALIA
- WOC pm 3:50 **Gas-Phase Conformations, Energetics, and Mechanisms for Glycosidic Bond Dissociation of Protonated 2'-Deoxycytidine and Cytidine;** Ranran Wu; Mary T. Rodgers; *Wayne State University, Detroit, MI*
- WOC pm 4:10 **New Insight into Ion/Molecule Chemistry with Isomeric Metal and Metal-Oxo Complexes using ESI-TWIMS-MS: C-F Bond-Activation, Active Species Structure and Mechanism;** Nicole Rijs; Maria Schlangen; Helmut Schwarz; *TU Berlin, Berlin, Germany*

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON  
NUCLEIC ACIDS**  
Valérie Gabelica (University of Bordeaux) presiding  
Room 120/127

- WOD pm 2:30 **A Proteomics-like Pipeline for the Epitranscriptome: Automated Analysis of Posttranscriptionally Modified RNAs;** Collin Wetzel; Patrick A. Limbach; *University of Cincinnati, Cincinnati, OH*
- WOD pm 2:50 **LC-MS/MS for Simultaneous Assessment of Oxidative DNA Adducts and a DNA Epigenetic Biomarker in an Animal Model of Wilson’s Disease;** Yang Yu; Candace R. Guerrero; Yinsheng Wang; *University of California, Riverside, Riverside, CA*



## WEDNESDAY AFTERNOON ORAL SESSIONS

- WOD pm 3:10 **Using Negative Mode ESI/MSMS to Sequence miRNAs and Detect Modifications**; Samuel Wein; Simone Sidoli; Benjamin A. Garcia; *University of Pennsylvania, Philadelphia, PA*
- WOD pm 3:30 **Structural Elucidation and Antisense Properties of a Sugar-Modified DNA Analogue**; Yvonne Hari; Christian Leumann; Stefan Schürch; *Department of Chemistry and Biochemistry, Bern, Switzerland*
- WOD pm 3:50 **Ion Mobility and Tandem Mass Spectrometry Reveal the Effects of Solution on Gas-phase RNA Hairpin Structure**; Kevin Ilek; Jessica Rabuck-Gibbons; Brandon Ruotolo; Kristina Hakansson; *University of Michigan, Ann Arbor, MI*
- WOD pm 4:10 **Discriminating Local Versus Global Dynamics in Structured Biopolymers by Ion Mobility Spectrometry-Mass Spectrometry**; Jennifer Lippens<sup>1</sup>; Rebecca D'Esposito<sup>1</sup>; Srivathsan Ranganathan<sup>1</sup>; Papa Nii Asare-Okai<sup>2</sup>; Daniele Fabris<sup>1</sup>; <sup>1</sup>*The RNA Institute, University at Albany, Albany, NY*; <sup>2</sup>*State University of New York at Albany, Albany, NY*

### 2:30 – 4:30 PM, WEDNESDAY AFTERNOON

#### FOOD CHEMISTRY AND SAFETY

**Timothy Croley (FDA) presiding**  
Theater

- WOE pm 2:30 **Beeromics: From QC to ID's of Differentially Expressed Compounds in Craft Beers**; Christine A. Hughey; Chelsey McMinn; Jenny Phung; *James Madison University, Harrisonburg, VA*
- WOE pm 2:50 **Evaluation of the Composition and Toxicity of Electronic Cigarette Liquids**; Sandra E. Spencer<sup>1</sup>; Rachel A. Harris<sup>1</sup>; Steven L. Reeber<sup>1</sup>; Phillip Clapp<sup>2</sup>; Ilona Jaspers<sup>2</sup>; Gary L. Glish<sup>2</sup>; <sup>1</sup>*UNC Chapel Hill, Department of Chemistry, Chapel Hill, NC*; <sup>2</sup>*UNC Chapel Hill, School of Medicine, Chapel Hill, NC*
- WOE pm 3:10 **Direct Identification of Prohibited Substances in Cosmetics Using a Miniature Mass Spectrometry System**; Qiang Ma<sup>1,2</sup>; R. Graham Cooks<sup>2</sup>; Zheng Ouyang<sup>2</sup>; <sup>1</sup>*Chinese Academy of Inspection and Quarantine, Beijing, China*; <sup>2</sup>*Purdue University, West Lafayette, IN*
- WOE pm 3:30 **Ambient Mass Spectrometry Imaging of Food Contaminants**; Michel W. Nielsen<sup>1,2</sup>; Wilco Duvivier<sup>2</sup>; Teris van Beek<sup>2</sup>; <sup>1</sup>*RIKILT-Institute of Food Safety, Wageningen, Netherlands*; <sup>2</sup>*Wageningen University, Wageningen, NL*
- WOE pm 3:50 **Identification of Biological Species using Spectral Libraries**; Magnus Palmblad<sup>1</sup>; Merel Nessen<sup>2</sup>; Tune Wulff<sup>3</sup>; Hans Dalebout<sup>1</sup>; Rob Marissen<sup>1</sup>; Dana Ohana<sup>1</sup>; Suzanne van der Plas-Duivestijn<sup>1</sup>; Arzu Tugce Guler<sup>1</sup>; Coen Mulders<sup>1</sup>; Sander Grevers<sup>1</sup>; Dennis van der Zwaan<sup>2</sup>; Alexandra Galitsyna<sup>1</sup>; Anastasia Stolyarova<sup>1</sup>; Martijn Staats<sup>2</sup>; Flemming Jessen<sup>3</sup>; Martha van der Beek<sup>1</sup>; Jeroen de Keijzer<sup>1</sup>; Peter van Veelen<sup>1</sup>; Michael Engelbrecht Nielsen<sup>3</sup>; Esther Kok<sup>2</sup>; Ed Kuijper<sup>1</sup>; Jonas Bergquist<sup>4</sup>; André Deelder<sup>1</sup>; <sup>1</sup>*Leiden University Medical Center, Leiden, Netherlands*; <sup>2</sup>*RIKILT Wageningen UR, Wageningen, Netherlands*; <sup>3</sup>*National Food Institute, Technical University of Denmark, Kgs. Lyngby, Denmark*; <sup>4</sup>*Uppsala University, Uppsala, Sweden*
- WOE pm 4:10 **Tracking Gluten Hydrolysis Throughout the Brewing Process**; Katherine L. Fiedler; Rakhi Panda; Whitney L. Stutts; Chung Y. Cho; Eric A.E. Garber; Timothy R. Croley; *CFSAN, U.S. FDA, College Park, MD*

### 2:30 – 4:30 PM, WEDNESDAY AFTERNOON H/D EXCHANGE: TECHNOLOGIES AND APPLICATIONS

**Derek Wilson (York University) presiding**  
Room 106

- WOF pm 2:30 **>95% Sequence Coverage within 10 Minutes for Structural Elucidation of Antibodies by Middle Down HDX/MS**; Jingxi Pan<sup>1</sup>; Suping Zhang<sup>1</sup>; Albert Chou<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>*University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada*; <sup>2</sup>*Dept. of Biochem. & Microbiol., Univ. of Victoria, Victoria, BC, Canada*
- WOF pm 2:50 **Temperature-dependent Conformational Dynamics in Whole Dengue Viral Particles by Hydrogen/Deuterium Exchange Mass Spectrometry**; Xin Xiang Lim; Arun Chandramohan; Ganesh S. Anand; *NUS Singapore, Singapore, Singapore*
- WOF pm 3:10 **Monte Carlo Simulations of Hydrogen Exchange Reveal Surprising Insights about the Isotopic Distribution**; David Weis; *University of Kansas, Lawrence, KS*
- WOF pm 3:30 **Exploring the Potential of Hydrogen-Deuterium Exchange Mass Spectrometry for Screening Protein/Ligand Interactions in Drug Discovery**; Haihong Zhou<sup>1</sup>; Robin Rolser<sup>1</sup>; Robert Myers<sup>1</sup>; Judyann Wiltsie<sup>1</sup>; Jose Castro-Perez<sup>1</sup>; David McLaren<sup>1</sup>; Stephen Previs<sup>1</sup>; George Addona<sup>2</sup>; Michael Kavana<sup>1</sup>; <sup>1</sup>*Merck & Co., Inc., Kenilworth, NJ*; <sup>2</sup>*Merck Co. & Inc., Boston, MA*
- WOF pm 3:50 **Electrochemical Reduction of Large and Highly Disulfide-Bonded Proteins – Complete Sequence Coverage in HDX-MS Experiments**; Esben Trabjerg<sup>1,2</sup>; Rasmus U. Jakobsen<sup>1</sup>; Simon Myslind<sup>3</sup>; Søren Christensen<sup>2</sup>; Thomas J.D. Jørgensen<sup>4</sup>; Kasper D. Rand<sup>1</sup>; <sup>1</sup>*Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark*; <sup>2</sup>*Biologics, H. Lundbeck A/S, Valby, Denmark*; <sup>3</sup>*Finsen Laboratory, Rigshospitalet and BRIC, Copenhagen, Denmark*; <sup>4</sup>*Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense, Denmark*
- WOF pm 4:10 **Investigating the Importance of Protein Conformational Dynamics During Catalysis by HDX-MS: Focus on the F<sub>1</sub>F<sub>0</sub>-ATP Synthase Molecular Machine**; Siavash Vahidi; Yumin Bi; Stanley Dunn; Lars Konermann; *Univ. of Western Ontario, London, CANADA*

### 2:30 – 4:30 PM, WEDNESDAY AFTERNOON

#### ENERGY, PETROLEUM, AND BIOFUELS: ADVANCES IN SAMPLE PREPARATION AND MS INTERFACE

**Mark P. Barrow (University of Warwick) presiding**  
Ballroom 222/224

- WOG pm 2:30 **Modern Petroleomics**; Ryan P. Rodgers<sup>1,2</sup>; Winston K. Robbins<sup>3</sup>; Jonathan Putman<sup>2</sup>; Vladislav Lobodin<sup>1,2</sup>; Priscila Lalli<sup>1,2</sup>; David Podgorski<sup>1,2</sup>; Steven Rowland<sup>1,2</sup>; Jie Lu<sup>2</sup>; Yuri Corilo<sup>1,2</sup>; Alan Marshall<sup>1,4</sup>; <sup>1</sup>*National High Magnetic Field Laboratory, Tallahassee, FL*; <sup>2</sup>*Future Fuels Institute, Tallahassee, FL*; <sup>3</sup>*Consultant, Brunswick, ME*; <sup>4</sup>*FSU Department of Chemistry and Biochemistry, Tallahassee, FL*
- WOG pm 2:50 **Monitoring the Photo Transformation of Crude Oils using SAIMS-FT-ICR MS**; Paolo Benigni<sup>1</sup>; Kathia Sandoval<sup>1</sup>; Christopher Thompson<sup>2</sup>; Mark Ridgeway<sup>3</sup>; Melvin A. Park<sup>3</sup>; Piero Gardinali<sup>1</sup>; Francisco Fernandez Lima<sup>1</sup>; <sup>1</sup>*Florida International University, Miami, FL*; <sup>2</sup>*Bruker Daltonics Inc., Billerica, MA*; <sup>3</sup>*Bruker Daltonics, Billerica, MA*





- WOG pm 3:10 **Petrochemical Isomer Distribution Analysis Using Cold EI GC/MS**; [Adam J. Patkin](#); Sharanya Reddy; Andrew N. Tyler; *PerkinElmer, Shelton, CT*
- WOG pm 3:30 **Lignomic Profiling of Extractives from Grasses using Electrospray Ionization and LC-TOFMS with Gamma-Valerolactone as a Renewable High-Boiling Mobile Phase**; [Afrand Kamali Sarvestani](#)<sup>1</sup>; <sup>3</sup>; Leonardo Da Costa Sousa<sup>2,3</sup>; Venkatesh Balan<sup>2,3</sup>; Bruce E. Dale<sup>2,3</sup>; A. Daniel Jones III<sup>1,3</sup>; *<sup>1</sup>Department of Chemistry, Michigan State University, East Lansing, MI; <sup>2</sup>Dept of Chemical Eng, Michigan State University, East Lansing, MI; <sup>3</sup>Great Lakes Bioenergy Research Center, East Lansing, MI*
- WOG pm 3:50 **Determination of the Average Molecular Weight of Crude Oil by Using Gas and Liquid Chromatography and Tandem Mass Spectrometry**; Ravikiran Yerabolu; [Raghavendhar Kotha](#); Xueming Dong; Hilikka Kenttamaa; *Purdue University, West Lafayette, IN*
- WOG pm 4:10 **Selective Chromatographic Separation of Crude Oil Mixtures by Online Coupling with Ultrahigh Resolution Mass Spectrometry**; [Wolfgang Schrader](#); Alessandro Vetere; Lilla Molnárné Guricza; *Max-Planck Inst für Kohlenforschung, Mülheim / Ruhr, GERMANY*

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON  
ANTIBODIES AND ANTI-BODY DRUG CONJUGATES**  
**Keyang Xu (Genentech, Inc.) presiding**  
**Ballroom 220/221**

- WOH pm 2:30 **Comprehensive Characterization of Three IgG Forms using CESI-MS**; [Bryan Fonslow](#)<sup>1</sup>; Olga V. Friese<sup>2</sup>; K. Steven Cook<sup>2</sup>; *<sup>1</sup>SCIEX, Brea, CA; <sup>2</sup>Pfizer, Chesterfield, MO*
- WOH pm 2:50 **In-depth Characterization of Lysine-Conjugated Antibody-Drug Conjugates (ADCs) by a Multiplexed MS/MS Data Acquisition Strategy Combined with Multi-Enzyme Digestion**; [Liuxi Chen](#)<sup>1</sup>; Robert Birdsall<sup>1</sup>; Henry Shion<sup>1</sup>; Ying-Qing Yu<sup>1</sup>; Frank Kotch<sup>2</sup>; April Xu<sup>3</sup>; Thomas Porter<sup>4</sup>; Weibin Chen<sup>1</sup>; *<sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Pfizer Bioprocess Research & Development, Pearl River, NY; <sup>3</sup>Pfizer Analytical Research & Development, Pearl River, NY; <sup>4</sup>Pfizer Analytical Research & Development, Andover, MA*
- WOH pm 3:10 **Antibody-Drug Conjugate (ADC) Bioanalysis by Immuno-capture LC-MS/MS Hybrid Assays: Challenges, Solutions and Complementarity with Ligand Binding Assays (LBA)**; [Jian Wang](#); Ang Liu; Huidong Gu; Frank Zambito; Alexander Kozhich; Heather Myler; Mark Arnold; Anne-Françoise Aubry; *Bristol-Myers Squibb, Princeton, NJ*
- WOH pm 3:30 **Improved Top-Down and Middle-Down Characterization of Complex Biopharmaceuticals on a Modified Tribrid Mass Spectrometer**; [Luca Fornelli](#)<sup>1</sup>; Philip D. Compton<sup>1</sup>; Seema Sharma<sup>2</sup>; Jesse D. Canterbury<sup>2</sup>; Christopher Mullen<sup>2</sup>; Vlad Zabrouskov<sup>2</sup>; Michael W. Senko<sup>2</sup>; Andrew P. Mazar<sup>1</sup>; Neil L. Kelleher<sup>1</sup>; *<sup>1</sup>Northwestern University, Evanston, IL; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA*
- WOH pm 3:50 **Dissecting the FcRn Binding Mode of Antibodies with Different Pharmacokinetic Profiles by Hydrogen/Deuterium Exchange Mass Spectrometry**; [Pernille Foged Jensen](#)<sup>1</sup>; Vincent Larraillet<sup>2</sup>; Angela Schoch<sup>2</sup>; Maximiliane Hilger<sup>2</sup>; Thomas Emrich<sup>2</sup>; Tilman Schlothauer<sup>2</sup>; Kasper D. Rand<sup>1</sup>; *<sup>1</sup>Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; <sup>2</sup>pRED, Roche Innovation Center, Penzberg, Germany*

- WOH pm 4:10 **Novel Sample Treatment and LC/MS Strategies Achieved Highly Accurate and Sensitive Investigation of Tissue Distributions of Therapeutic Monoclonal Antibody**; [Ming Zhang](#); Bo An; Haoying Yu; Jun Qu; *SUNY at Buffalo, Buffalo, NY*

**4:45 – 5:30 PM, WEDNESDAY AFTERNOON  
ASMS MEETING**  
**Jenny Brodbelt, ASMS President, presiding**  
**Enjoy a beverage and hear the latest ASMS news.**  
**Ballroom 222/224, level 2**

**5:45 – 7:00 PM, WEDNESDAY AFTERNOON  
WORKSHOPS**  
There are light refreshments in the common areas.

01. The role of High Resolution Mass Spectrometry in the Regulatory Environment, Room 130
02. Emerging Contaminants for Emerging Scientists, Room 131
03. Mass spectrometry instrumentation at the forefront of technology as miscible tools for forensic and security evidence, Room 132
04. Gas-phase ion chemistry: thermodynamics, kinetics, structures and spectroscopy, Room 123/124
05. Emerging Technologies Advancing Mass Spectrometry Research: 3D Printing, Room 120/127
06. CHORUS - A community solution for the Storage Visualization, Sharing, and Analysis of Mass Spectrometry Data on the Cloud, Room 260/267
07. The Big Fat Questions: Tthe future for lipidomics in cell biology and clinical diagnostics? Room 274
08. Characterization of Protein Therapeutics by Mass Spectrometry, Room 275
09. Getting the Most out of Undergraduate Research in Mass Spectrometry, Room 230
10. Working with Federal Agencies to Obtain Research Support: Mock NIH Study Section and Q&A with Agency Staff, Room 231
11. Room 232
12. Ligand Binding Assays (LBA) and LC-MS/MS Integrated Antibody-Drug Conjugate (ADC) Bioanalysis -Immuno-capture LC-MS/MS Hybrid Assays: Challenges, Solutions, and Complementarity with LBA, Ballroom 222/224
13. Hydrogen-Deuterium Exchange, Covalent Labeling and Crosslinking, Ballroom 220/221

**AFTER 8:00 PM  
CORPORATE HOSPITALITY SUITES  
RENAISSANCE GRAND HOTEL**



**8:30 – 10:30 AM, THURSDAY MORNING  
MINI/OORTABLE/FIELDABLE MS  
Zheng Ouyang (Purdue University) presiding  
Hall 5**

- ThOA am 08:30 **Investigation of NIR Diode Wavelength and Material Combinations for Increased Permeability in Portable Membrane Inlet Mass Spectrometry;** Phillip Mach<sup>1</sup>; Kenneth Wright<sup>2</sup>; Guido Verbeck<sup>1</sup>; <sup>1</sup>University of North Texas, Denton, TX; <sup>2</sup>Inficon, Syracuse, NY
- ThOA am 08:50 **Chemical Ionization Mass Spectrometry Using Carbon Nanotube Field Emission Electron Sources;** Erich Radauscher<sup>1</sup>; Adam Keil<sup>2</sup>; Mitch Wells<sup>2</sup>; Jason Amsden<sup>1</sup>; Jeffrey Piascik<sup>3</sup>; Charles Parker<sup>1</sup>; Brian Stoner<sup>3</sup>; Jeffrey Glass<sup>1</sup>; <sup>1</sup>Duke University, Durham, NC; <sup>2</sup>FLIR Systems, West Lafayette, IN; <sup>3</sup>Engineering and Applied Physics Division, RTI Int, Research Triangle Park, NC
- ThOA am 09:10 **Rarefied Choked Flow in a Microscale Ion Trap Operated at High Pressure;** Bruno Coupier; Kevin Schultze; Sorin Mitran; J. Michael Ramsey; *UNC Chapel Hill, Chapel Hill, NC*
- ThOA am 09:30 **Old Dog, New Tricks: Enhanced Quadrupole Performance by Addition of a Magnetic Field;** Simon Maher<sup>1,2</sup>; Sarfaraz U. A. Syed<sup>3</sup>; John R. Gibson<sup>2</sup>; Fred P. M. Jjunju<sup>2</sup>; Barry L. Smith<sup>4</sup>; David Taylor<sup>4</sup>; Iain S. Young<sup>1</sup>; Ron M. A. Heeren<sup>3</sup>; Stephen Taylor<sup>2</sup>; <sup>1</sup>Institute of Integrative Biology, University of Liverpool, UK; <sup>2</sup>Dept. of Electrical Engineering and Electronics, University of Liverpool, UK; <sup>3</sup>FOM Institute for Atomic and Molecular Physics, Amsterdam, Netherlands; <sup>4</sup>Q Technologies, Liverpool, UK
- ThOA am 09:50 **A Mini-Mass Spectrometer with Continuous Atmospheric Pressure Interface: Pushing the Limits of Ion Transfer Device, Vacuum System and Ion Trap;** Yanbing Zhai; Muyi He; Yongzheng Wei; Wei Xu; *Beijing Institute of Technology, Beijing, CHINA*
- ThOA am 10:10 **Development of Portable Particle Mass Spectrometer with Ambient Aerodynamic Ion Source;** Caiqiao xiong<sup>1</sup>; Yiming Zhang<sup>2</sup>; Suming Chen<sup>1</sup>; Zongxiu Nie<sup>1</sup>; <sup>1</sup>Institute of Chemistry Chinese Academy of Sciences, Beijing, China; <sup>2</sup>Jiangsu Skyray Instrument Inc., Suzhou, Kunshan

**8:30 – 10:30 AM, THURSDAY MORNING  
INFORMATICS: PEPTIDE IDENTIFICATION AND QUANTIFICATION  
William Noble (University of Washington) presiding  
Room 130/132**

- ThOB am 08:30 **Machine Learning Approach for Inferring Atomic Composition of Peptides from Peaks with Unresolved Isotopic Fine Structure;** Tikira Temu<sup>1</sup>; Annette Michalski<sup>1,2</sup>; Stefka Tyanova<sup>1</sup>; Matthias Mann<sup>1</sup>; Juergen Cox<sup>1</sup>; <sup>1</sup>Max-Planck Institute of Biochemistry, Martinsried, DE; <sup>2</sup>Bruker Daltonik GmbH, Bremen, DE
- ThOb am 08:50 **Fast and Accurate Unrestricted Spectrum Interpretation: You Don't Know What You're Missing;** Arun Devabhaktuni; Josh Elias; *Stanford University, Stanford, CA*
- ThOB am 09:10 **De novo Sequencing using MELD Proteolysis Coupled to a "Sequence Assembly" Algorithm;** Gabriel Mazzucchelli<sup>1</sup>; Tyler A Zimmerman<sup>2</sup>; Nicolas Smargiasso<sup>1</sup>; Dominique Baiwir<sup>3</sup>; Marie-Alice Meuwis<sup>4</sup>; Edwin De Pauw<sup>1</sup>; <sup>1</sup>Univeristy of Liege, MS Lab - GIGA, Liege, Belgium; <sup>2</sup>National Institute of Standards and Technology, Gaithersburg, MD; <sup>3</sup>University of Liege, GIGA-Proteomics, Liege, Belgium; <sup>4</sup>CHU, Gastroenterology unit, Liege, Belgium

- ThOB am 09:30 **Isobaric Labeling Assisted Proteome Identification and Quantification Based on Database Search and Denovo Sequencing;** Yichu Shan<sup>1</sup>; Shen Zhang<sup>1,2</sup>; Lihua Zhang<sup>1</sup>; Yukui Zhang<sup>1</sup>; <sup>1</sup>Dalian Institute of Chemical Physics, dalian, china; <sup>2</sup>Univiersity of Chinese Academy of Sciences, Beijing, china
- ThOB am 09:50 **Increasing Depth of Proteomic Profiling in MS Data-Dependent Acquisition (DDA) Discovery Experiments Using Advanced Precursor Ion Selection Algorithms;** Simion Kreimer<sup>1</sup>; William Danielson<sup>2</sup>; Mikhail Belov<sup>2</sup>; Barry Karger<sup>1</sup>; Alexander R. Ivanov<sup>1</sup>; <sup>1</sup>Barnett Inst., Northeastern University, Boston, MA; <sup>2</sup>Spectrograph LLC, Kennewick, WA
- ThOB am 10:10 **Accurate and Rapid Quantification of Co-Eluting Deamidated and Non-Deamidated Peptides using a Novel Deconvolution Technique;** Yong Kil<sup>1</sup>; Marshall W. Bern<sup>1</sup>; Eric Carlson<sup>1</sup>; Chris Becker<sup>1</sup>; David Morgenstern<sup>2</sup>; Beatrix Ueberheide<sup>2</sup>; <sup>1</sup>Protein Metrics Inc., San Carlos, CA; <sup>2</sup>NYU School of Medicine, New York City, NY

**8:30 – 10:30 AM, THURSDAY MORNING  
NEW AND DEVELOPING ION ACTIVATION METHODS  
Kaveh Jorabchi (Georgetown University) presiding  
Room 123/124**

- ThOC am 08:30 **Enhancement of Ion Activation and CID by Simultaneous Dual Dipolar Excitation in X and Y Directions in Linear Ion Trap;** Xiao Dong Xie<sup>1</sup>; Qiankun Dang<sup>1</sup>; Fuxing Xu<sup>1</sup>; Xinhua Dai<sup>2</sup>; Xiang Fang<sup>2</sup>; Chuan-Fan Ding<sup>1</sup>; <sup>1</sup>Fudan University, Shanghai, China; <sup>2</sup>National Institute of Metrology, Beijing, China
- ThOC am 08:50 **Charge Transfer Dissociation (CTD) Mass Spectrometry;** Glen Jackson; William Hoffmann; *West Virginia University, Morgantown, WV*
- ThOC am 09:10 **High-Energy (> 50 eV) Electron-Induced Dissociation of Therapeutic Drugs in a QTOF Mass Spectrometer;** Yury V Vasil'ev; Valery G. Voinov; Samuel E. Bennett; Joseph S. Beckman; Douglas F. Barofsky; *Oregon State University, Corvallis, OR*
- ThOC am 09:30 **Ultraviolet Photodissociation for Analysis of Native Proteins, Protein Complexes, and Charge-Reduced Proteins in the Gas Phase;** Dustin Holden<sup>2</sup>; Jennifer Brodbelt<sup>1</sup>; <sup>1</sup>The University of Texas, Austin, TX; <sup>2</sup>University of Texas Chemistry, Austin, TX
- ThOC am 09:50 **Interrogation of Protein Structure using Conformer Selection, VUPD, and ETnod;** Bruno Bellina<sup>1</sup>; Jeff Brown<sup>2</sup>; Jakub Ujma<sup>1</sup>; Kevin Giles<sup>2</sup>; Paul Murray<sup>2</sup>; Rebecca Beveridge<sup>1</sup>; Eleanor Dickinson<sup>1</sup>; Jonathan P. Williams<sup>2</sup>; Mike Morris<sup>2</sup>; Perdita Barran<sup>1</sup>; <sup>1</sup>The University of Manchester, Manchester, UK; <sup>2</sup>Waters Corporation, Wilmslow, UK
- ThOC am 10:10 **Efficient and Selective Covalent Bond Formation between Peptide Ion Dimers Using 355 nm Light;** Christopher Shaffer; Andy Dang; Emilie Viglino; Frantisek Turecek; *University of Washington, Seattle, Washington*

**8:30 – 10:30 AM, THURSDAY MORNING  
NEW NANO-SCALE AND MICROFLUIDIC  
SEPARATIONS AND MS  
Liangliang Sun (University of Notre Dame) presiding  
Room 120/127**

- ThOD am 08:30 **A Handheld Ultrafast CE Interfaced to MS for the Analysis of Explosives, Illicit Drugs, Amino Acids and their Optical Isomers;** Mehdi Moini; Christopher Rollman; *George Washington University, Washington, DC*



ThOD am 08:50 **Identification of Metabolites in Crustacean Hemolymph via *in vivo* Microdialysis by Capillary Electrophoresis-Matrix-Assisted Laser Desorption/Ionization Mass Spectrometric Imaging Platform;** Shan Jiang; Zhidan Liang; Lingjun Li; *UW-Madison, Madison, WI*

ThOD am 09:10 **Development, Characterization and Application of Slug Flow Microextraction (SFME) for Direct MS Analysis of Biological Samples;** Yue Ren; Zheng Ouyang; *Purdue University, West Lafayette, IN*

ThOD am 09:30 **Microchip Capillary Electrophoresis with Integrated Electrospray Ionization for Rapid and Efficient Analysis of Polar Metabolites in Biological Samples;** J. Scott Mellors<sup>1</sup>; Michael Pacold<sup>2</sup>; Elizaveta Freinkman<sup>3</sup>; Erin Redman<sup>2</sup>; J. Michael Ramsey<sup>2</sup>; <sup>1</sup>908 Devices Inc., Boston, MA; <sup>2</sup>University of North Carolina, Chapel Hill, NC; <sup>3</sup>Whitehead Institute for Biomedical Research, Cambridge, MA

ThOD am 09:50 **Development of High Sensitivity Intact Monoclonal Antibody (mAb) Analysis Using an Integrated Microfluidics MS System;** Gregory Roman; Henry Shion; Weibin Chen; James Murphy; *Waters Corporation, Milford, MA*

ThOD am 10:10 **Analysis of Proteins, Protein Complexes and Proteomes under Non-Denaturing Conditions Using Sheathless Capillary Electrophoresis Coupled with Native Mass Spectrometry;** Alexander R. Ivanov<sup>1</sup>; Rosa Viner<sup>2</sup>; Marcia R. Santos<sup>3</sup>; Arseniy M. Belov<sup>1</sup>; Chitra K. Ratnayake<sup>3</sup>; David M. Horn<sup>4</sup>; Marshall W. Bern<sup>5</sup>; Barry L. Karger<sup>1</sup>; <sup>1</sup>Barnett Inst., Northeastern University, Boston, MA; <sup>2</sup>ThermoFisher Scientific, San Jose, CA; <sup>3</sup>Sciex, Brea, CA; <sup>4</sup>Thermo Fisher Scientific, San Jose, CA; <sup>5</sup>Protein Metrics, Palo Alto, CA

**8:30 – 10:30 AM, THURSDAY MORNING  
STRUCTURE/REACTIVITY AND ENERGETICS OF  
GAS-PHASE IONS AND COMPLEXES  
Ken Ervin (University of Nevada, Reno) presiding  
Theater**

ThOE am 08:30 **Gas-Phase Reactivity of Phenoxy Radical Cations of Tyrosine and Related Model Compounds;** Michael Lesslie<sup>1</sup>; Andrii Piatkivskiy<sup>1</sup>; Sandra Osburn<sup>2</sup>; Richard A. J. O'Hair<sup>2</sup>; Victor Ryzhov<sup>1</sup>; <sup>1</sup>Northern Illinois University, Dekalb, IL; <sup>2</sup>University of Melbourne, Melbourne, Australia

ThOE am 08:50 **The Effects of Protonation vs Noncovalent Interactions with Sodium Cations on the Structures and Stability of DNA and RNA Nucleosides;** Mary T. Rodgers<sup>1</sup>; Ranran Wu<sup>1</sup>; Yanlong Zhu<sup>1</sup>; Chenchen He<sup>1</sup>; Stephen Strobehn<sup>1</sup>; Juehan Gao<sup>2</sup>; Jos Oomens<sup>2</sup>; <sup>1</sup>Wayne State University, Detroit, MI; <sup>2</sup>Radboud University Nijmegen, Nijmegen, NETHERLANDS

ThOE am 09:10 **Gas-Phase Reactions of Ionic Liquid Anions;** Charles Nichols<sup>1,2</sup>; W. Carl Lineberger<sup>1,2</sup>; Veronica M. Bierbaum<sup>1,2</sup>; <sup>1</sup>University of Colorado, Boulder, CO; <sup>2</sup>JILA, Boulder, Colorado

ThOE am 09:30 **Pushing it to the Red: Probing the Influence of Ligands on the Antisymmetric Uranyl Stretching Frequency using IRMPD Spectroscopy;** Michael J. Van Stipdonk<sup>1</sup>; John Gibson<sup>2</sup>; Bert De Jong<sup>2</sup>; Phuong Dau<sup>2</sup>; Giel Gerden<sup>3</sup>; Jos Oomens<sup>3</sup>; <sup>1</sup>Duquesne University, Pittsburgh, PA; <sup>2</sup>Lawrence Berkeley Nat'l Lab, Berkeley, CA; <sup>3</sup>Radboud University Nijmegen, Nijmegen, Netherlands

ThOE am 09:50 **Water-Network Mediated, Electron Induced Proton Transfer in Anionic [C<sub>2</sub>H<sub>5</sub>N<sup>+</sup>(H<sub>2</sub>O)<sub>n</sub>]<sup>-</sup> Clusters: Size-Dependent Formation of the Pyridinium Radical for n ≥ 3;** Andrew F. DeBlase<sup>1,4</sup>; Gary H. Weddle<sup>2,4</sup>; Kaye A. Archer<sup>3</sup>; Kenneth D. Jordan<sup>3</sup>; Mark A. Johnson<sup>4</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>Fairfield University, Fairfield, CT; <sup>3</sup>University of Pittsburgh, Pittsburgh, PA; <sup>4</sup>Yale University, New Haven, CT

ThOE am 10:10 **Disentangling Reactive Isomers in Combustion Chemistry using Photoelectron Photoion Coincidence Spectroscopy;** Tina Kasper<sup>1</sup>; Thomas Bierkandt<sup>1</sup>; Patrick Oßwald<sup>2</sup>; Markus Köhler<sup>2</sup>; Patrick Hemberger<sup>3</sup>; <sup>1</sup>Thermodynamics, University of Duisburg-Essen, Duisburg, Germany; <sup>2</sup>DLR – Institute of Combustion Technology, Stuttgart, Germany; <sup>3</sup>Molecular Dynamics Group, SLS, Paul Scherrer Inst., Villigen, Switzerland

**8:30 – 10:30 AM, THURSDAY MORNING  
MS IN PROTEIN FOOTPRINTING:  
MICHAEL GROSS 75TH BIRTHDAY  
Ragu Ramanathan and  
Christopher L. Holiman (Pfizer, Inc.) presiding  
Room 106**

ThOF am 08:30 **Review of Fast PhotoChemical Oxidative Footprinting Development in the Gross Lab;** David Hambly; *Amgen Inc., Longmont, CO*

ThOF am 08:50 **In Cell Protein Footprinting for the Analysis of Protein Structure;** Lisa M. Jones; *Indiana University-Purdue University Indianapolis, Indianapolis, IN*

ThOF am 09:10 **Mass Spectrometry for Probing Protein Higher Order Structure: An Industry Perspective;** Guodong Chen; Richard Huang; Hui Wei; Ekaterina Deyanova; Bethanne Warrack; Adrienne Tymiak; *Bristol-Myers Squibb, Princeton, NJ*

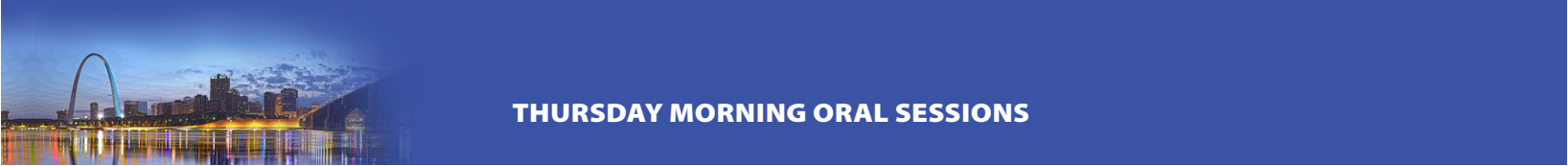
ThOF am 09:30 **Fast Photochemical Oxidation of Proteins (FPOP) Reveals the Binding Interface of an Antigen and Antibody;** Ying Zhang<sup>1</sup>; Aaron Weckler<sup>2</sup>; Patricia Molina<sup>2</sup>; Galahad Deperalta<sup>2</sup>; Michael L. Gross<sup>1</sup>; <sup>1</sup>Washington University in St. Louis, St. Louis, MO; <sup>2</sup>Genentech Inc., South San Francisco, CA

ThOF am 09:50 **Protein Footprinting for Quantitative Topography Analysis of Protein Structure;** Mark Chance; Janna Kiselar; Parminder Kaur; *Case Western Reserve University, Cleveland, OH*

ThOF am 10:10 **HDX, FPOP, and Specific Amino-acid Labeling are Complementary Methods for MS-based Protein Footprinting;** Michael L. Gross; *Washington University, St Louis, MO*

**8:30 – 10:30 AM, THURSDAY MORNING  
TARGETED QUANTIFICATION OF PROTEINS AND  
POST-TRANSLATIONAL MODIFICATIONS  
Birgit Schilling (Buck Institute for Research on Aging) presiding  
Ballroom 222/224**

ThOG am 08:30 **Proteoform Reaction Monitoring by Top-Down Proteomics: Moving from Discovery to Targeted Validation of Intact Protein Biomarkers;** Timothy K. Toby<sup>1</sup>; Luca Fornelli<sup>1</sup>; Kyunggon Kim<sup>1</sup>; Michael M. Abecassis<sup>2</sup>; Daniel R. Salomon<sup>3</sup>; Neil L. Kelleher<sup>1</sup>; <sup>1</sup>Northwestern University, Evanston, IL; <sup>2</sup>Northwestern Feinberg School of Medicine, Chicago, IL; <sup>3</sup>The Scripps Research Institute, La Jolla, CA



## THURSDAY MORNING ORAL SESSIONS

ThOG am 08:50 **Ubiquitin Ser65 Phosphorylation Affects Ubiquitin Structure, Chain Assembly and Hydrolysis**; Kirby Swatek; Tobias Wauer; Jane Wagstaff; Christina Gladkova; Jonathan Pruneda; Martin Michel; Malte Gersch; Christopher Johnson; Stefan Freund; David Komander; *MRC Laboratory of Molecular Biology, Cambridge, UK*

ThOG am 09:10 **Refinement of Parallel Reaction Monitoring Methods to Improve Accuracy in Peptide Quantification**; Sebastien Gallien; Daniel Ayoub; Sang Yoon Kim; Antoine Lesur; Bruno Doman; *Luxembourg Clinical Proteomics Center, Strassen, LUXEMBOURG*

ThOG am 09:30 **Optimized Protocol for MRM-based Protein Quantification in Archived Cancer Tissues**; Jacob Kennedy<sup>1</sup>; Regine Schoenherr<sup>1</sup>; Ping Yan<sup>1</sup>; Jeff Whiteaker<sup>1</sup>; Richard Ivey<sup>1</sup>; Melissa Lerch<sup>2</sup>; Geoffrey Baird<sup>2</sup>; Andy Hoofnagle<sup>2</sup>; Amanda Paulovich<sup>1</sup>; <sup>1</sup>*Fred Hutchinson Cancer Research Center, Seattle, WA*; <sup>2</sup>*UW Dept of Laboratory Medicine, Seattle, WA*

ThOG am 09:50 **Using Targeted Proteomics to Characterize the Relative Distribution of Apolipoprotein E Allele-Specific Isoforms in Clinically-Relevant Matrices**; James G. Bollinger<sup>1</sup>; Han-Yin Yang<sup>1</sup>; Clark Henderson<sup>1</sup>; Nicole Kuderer<sup>1</sup>; Christine Wu<sup>2</sup>; C. Anthony Blau<sup>1</sup>; Andrew Hoofnagle<sup>1</sup>; Michael MacCoss<sup>1</sup>; <sup>1</sup>*University of Washington, Seattle, WA*; <sup>2</sup>*Stratus Biosciences, Seattle, WA*

ThOG am 10:10 **From Discovery Proteomics to Targeted Biomarker Assays: Identification of Tau Post-Translational Modifications that Track O-GlcNAcase inhibition by Thiamet G**; Nathan G. Hatcher<sup>1</sup>; Ronald A. Miller<sup>1</sup>; Zhenlian Ke<sup>1</sup>; Julie Lee<sup>2</sup>; Helene L. Cardasis<sup>3</sup>; Giuseppe Terracina<sup>2</sup>; Lili Zhang<sup>4</sup>; Jacob Marcus<sup>1</sup>; Xiaohai Wang<sup>1</sup>; Dawn M. Toolan<sup>1</sup>; Bonnie J. Howell<sup>1</sup>; John J. Renger<sup>1</sup>; Sean M. Smith<sup>1</sup>; Daniel S. Spellman<sup>1</sup>; <sup>1</sup>*Merck Research Labs, West Point, PA*; <sup>2</sup>*Merck Research Labs, Kenilworth, NJ*; <sup>3</sup>*Thermo Fisher Scientific, Cambridge, MA*; <sup>4</sup>*Novartis Institute for Biomedical Research, Cambridge, MA*

### 8:30 – 10:30 AM, THURSDAY MORNING ION MOBILITY: SMALL MOLECULES, PHARMACEUTICALS AND DMPK

Erkinjon Nazarov (University of South Florida) presiding  
Ballroom 220-221

ThOH am 08:30 **Potential for Ion Mobility Spectrometry in Small Molecule Chiral Analysis**; Tawnya Flick; Iain D G Campuzano; Michael D Bartberger; *Amgen Inc., Thousand Oaks, CA*

ThOH am 08:50 **Separation of Isomeric Steroids using Ion Mobility QTOF-LC/MS**; Christopher D. Chouinard<sup>1</sup>; Christopher R. Beekman<sup>1</sup>; Timothy J. Garrett<sup>2</sup>; Richard A. Yost<sup>1</sup>; <sup>1</sup>*Department of Chemistry, University of Florida, Gainesville, FL*; <sup>2</sup>*Department of Pathology, University of Florida, Gainesville, FL*

ThOH am 09:10 **Collision Cross Section Calibration Strategies for Traveling-Wave Ion Mobility - Mass Spectrometry in Negative-Ion Mode**; Jay Forsythe<sup>1,2</sup>; Chelsea Walker<sup>1,2</sup>; Anton Petrov<sup>1,2</sup>; Samuel Allen<sup>3</sup>; Matthew Bush<sup>3</sup>; Nicholas Hud<sup>1,2</sup>; Facundo Fernandez<sup>1,2</sup>; <sup>1</sup>*Georgia Tech, School of Chemistry and Biochemistry, Atlanta, GA*; <sup>2</sup>*NSF/NASA Center for Chemical Evolution, Atlanta, GA*; <sup>3</sup>*University of Washington, Department of Chemistry, Seattle, WA*

ThOH am 09:30 **Comprehensive Screening and Characterisation of Metabolites and Biomolecules by Collisional Cross Section using a Novel Geometry Travelling-Wave IMS-QToF Mass Spectrometer**; Richard Gallagher<sup>1</sup>; Christine Pattison<sup>1</sup>; Kathryn Pickup<sup>1</sup>; Nick Tomczyk<sup>2</sup>; Martin Palmer<sup>2</sup>; Jason Wildgoose<sup>2</sup>; Darren Hewitt<sup>2</sup>; Daniel Weston<sup>2</sup>; <sup>1</sup>*Astrazeneca, Macclesfield, UK*; <sup>2</sup>*Waters, Wilmslow, UK*

ThOH am 09:50 **Ultra-Fast Separation and Quantification of Isobaric Barbiturates in Serum using LDTD-MS/MS Combined with Differential Mobility Spectrometry**; Sylvain Letarte; Alex Birsan; Serge Auger; Jean Lacoursière; Pierre Picard; *Phytronix Technologies, Inc., Quebec, Canada*

ThOH am 10:10 **Application of Differential Mobility Spectrometry Coupled with Multiple Ion Monitoring for Quantitation of Peptides Not Suited for MRM Analysis**; Yuan-Qing Xia<sup>1</sup>; Eugene Ciccimaro, Jr<sup>2</sup>; Naiyu Zheng<sup>2</sup>; Mingshe Zhu<sup>2</sup>; <sup>1</sup>*Sciex, Framingham, MA*; <sup>2</sup>*Bristol-Myers Squibb Company, Lawrenceville, NJ*

10:30 AM – 2:30 PM, THURSDAY  
THURSDAY POSTER SESSION  
Poster/Exhibit Hall  
Lunch concessions are open 11:00 am – 2:00 pm





2:30 – 4:30 PM, THURSDAY AFTERNOON  
MS IN SURGERY

Zoltan Takats (Imperial College London) presiding  
Hall 5

- ThOA pm 2:30 **Development of a System for the Investigation of Near Real-Time Tissue Identification Using Rapid Evaporative Ionisation Time-of-Flight Mass Spectrometry.**; Steven Pringle<sup>1</sup>; Julia balog<sup>2</sup>; Emrys A Jones<sup>1</sup>; Tamas Karancsi<sup>2</sup>; Keith Richardson<sup>1</sup>; Mike Morris<sup>1</sup>; <sup>1</sup>Waters Corporation, Wilmslow, United Kingdom; <sup>2</sup>Waters Research Center, Budapest, Hungary
- ThOA pm 2:50 **Ambient Ionization MS for Rapid Tissue Diagnosis During Surgical Intervention of Human Brain Cancer.**; Alan Jarmusch<sup>1</sup>; Valentina Pirro<sup>1</sup>; Zane Baird<sup>1</sup>; Clint Alfaro<sup>1</sup>; Eyas Hattab<sup>2</sup>; Aaron Cohen-Gadol<sup>3</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University-Department of Chemistry, West Lafayette, IN; <sup>2</sup>Department of Pathology, IUSM, Indianapolis, IN; <sup>3</sup>Department of Neurological Surgery, IUSM, Indianapolis, IN
- ThOA pm 3:10 **Chemical Biopsy based on SPME Approach: A New Medical Tool.**; Janusz Pawliszyn<sup>1</sup>; Barbara Bojko<sup>1</sup>; German Augusto Gomez-Rios<sup>1</sup>; Krzysztof Gorynski<sup>1</sup>; Jan Matthias Knaak<sup>2</sup>; Tiago Machuca<sup>3</sup>; Erasmus Cudjoe<sup>1</sup>; Vinzent Spetzler<sup>2</sup>; Michael Hsin<sup>3</sup>; Markus Selzner<sup>2</sup>; Mingyao Liu<sup>3</sup>; Marcelo Cypel<sup>3</sup>; Shaf Keshavjee<sup>3</sup>; <sup>1</sup>University of Waterloo, Waterloo, Canada; <sup>2</sup>Department of Surgery, Toronto General Hospital, Toronto, Canada; <sup>3</sup>University Health Network, University of Toronto, Toronto, Canada
- ThOA pm 3:30 **Endometriosis Foci Differentiation by Direct High Resolution Mass Spectrometry Methods.**; Alexey Kononikhin<sup>1, 4</sup>; Anna Bugrova<sup>1, 3</sup>; Natalia Starodubtseva<sup>1, 2</sup>; Anna Borisova<sup>1</sup>; Denis Bormotov<sup>4</sup>; Yury Kostyukevich<sup>2</sup>; Vladimir Naumov<sup>1</sup>; Igor Popov<sup>4</sup>; Vladimir Frankevich<sup>1</sup>; A. V. Kozachenko<sup>1</sup>; E. A. Kogan<sup>1</sup>; Leila V. Adamyan<sup>1</sup>; Gennady T. Sukhikh<sup>1</sup>; Eugene Nikolaev<sup>2, 4</sup>; <sup>1</sup>Research Center for Obstetrics, Gynecology, Moscow, Russia; <sup>2</sup>Institute for Energy Problems of Chemical Physics, Moscow, Russia; <sup>3</sup>Emanuel Institute of Biochemical Physics, Moscow, Russia; <sup>4</sup>Moscow Institute of Physics and Technology, Moscow, Russia
- ThOA pm 3:50 **Molecular Assessment of Gastric and Pancreatic Cancer Surgical Margins by Ambient Mass Spectrometry Imaging.**; Livia S. Eberlin; Robert Tibshirani; Katy Margulis-Goshen; Ivette Planell-Mendez; Moe Jalali; Teri A. Longacre; George A. Poultsides; Richard N. Zare; *Stanford University, Stanford, CA*
- ThOA pm 4:10 **Development of a Novel Instrument for ex-vivo and in-vivo Real-Time Analysis.**; Benoit Fatou<sup>1</sup>; Maxence Wisztorski<sup>1</sup>; Cristian Fosca<sup>2</sup>; Michael Ziskind<sup>2</sup>; Michel Salzet<sup>1</sup>; Isabelle Fournier<sup>1</sup>; <sup>1</sup>INSERM U1192 PRISM - University of Lille, Villeneuve d'Ascq, France; <sup>2</sup>CNRS UMR 8523 PhLAM - University of Lille, Villeneuve d'Ascq, France

2:30 – 4:30 PM, THURSDAY AFTERNOON  
MULTI-PTMS: COMPREHENSIVE ANALYSIS

Leslie M. Hicks (University of North Carolina, Chapel Hill) presiding  
Room 130/132

- ThOB pm 2:30 **Comprehensive Discovery of Protein Post-translational Modifications in Proteomic Datasets.**; Michael R. Shortreed<sup>1</sup>; Qiyao Li<sup>1</sup>; Brian L. Frey<sup>1</sup>; Craig D. Wenger<sup>2</sup>; Mark Scafl<sup>1</sup>; Lloyd M. Smith<sup>1</sup>; <sup>1</sup>University of Wisconsin, Madison, WI; <sup>2</sup>Unaffiliated, North Branford, CT

- ThOB pm 2:50 **Peptide Variant Discovery in Lens Tissue using Penalty-Based Spectral Alignment.**; Laurence E. Bernstein; Nuno Bandeira; *University of California, San Diego, La Jolla, CA*
- ThOB pm 3:10 **Complete Characterization of the Protein Post-Translational Modification Profiles through Combination of Native and Bottom-Up Mass Spectrometry.**; Fan Liu; Yang Yang; Albert J.R. Heck; *Utrecht University, Utrecht, The Netherlands*
- ThOB pm 3:30 **Tracing Protein Post-Translational Modifications at Different Growth Stages of the Archaeon *Sulfolobus islandicus* with Bottom-Up and Top-Down Proteomics.**; Egor Vorontsov; Elena Rensen; David Prangishvili; Mart Krupovic; Julia Chamot-Rooke; *Institut Pasteur, Paris, France*
- ThOB pm 3:50 **A Bottom-Up Informed Top-Down Approach Provides Insights into the Ubiquitin Code of Immune Cell Signaling.**; Giuseppe Infusini; Thomas Nebel; John Silke; Andrew Webb; *The Walter & Eliza Hall Institute, Parkville, Australia*
- ThOB pm 4:10 **Sirtuin 4 is a Lipoamidase Regulating Pyruvate Dehydrogenase Complex Activity.**; Rommel Mathias; Todd M. Greco; Adam Oberstein; Hanna Budayeva; Rumela Chakrabarti; Elizabeth Rowland; Yibin Kang; Thomas Shenk; Ileana M. Cristea; *Princeton University, Princeton, NJ*

2:30 – 4:30 PM, THURSDAY AFTERNOON  
PEPTIDE FRAGMENTATION AND PEPTIDOMICS

Carlito Lebrilla (University of California, Davis) presiding  
Room 123/124

- ThOC pm 2:30 **Analytic Framework for Peptidomics Applied to Large-Scale Neuropeptide Identification.**; Christian Kelstrup; Anna Secher<sup>2</sup>; Jesper V. Olsen<sup>1</sup>; <sup>1</sup>NNF CPR, University of Copenhagen, Copenhagen, Denmark; <sup>2</sup>Novo Nordisk, Måløv, Denmark
- ThOC pm 2:50 **Ion Mobility Peptidomic Analysis of Endogenous Peptides Reveals Functions through Conformations.**; Andres Guerrero<sup>1</sup>; Miguel Angel Garcia Mompean<sup>2</sup>; Cassandra Yee<sup>1</sup>; David Wong<sup>3</sup>; Carlito Lebrilla<sup>1</sup>; <sup>1</sup>UC Davis, Chemistry Department, Davis, CA; <sup>2</sup>Institute of Physical Chemistry Rocasolano, CSIC, Madrid, Spain; <sup>3</sup>Agilent Technologies, Inc., Santa Clara, CA
- ThOC pm 3:10 **Lymph-Carried Self-Antigens Derive from a Variety of Processing Enzymes and Contribute to the Dendritic Cells MHC II Peptidome.**; Cristina Clement<sup>1</sup>; Aniuska Becerra<sup>2</sup>; Liusong Yin<sup>2</sup>; Valerio Zolla<sup>1</sup>; Scott Shafer<sup>2</sup>; Lawrence J. Stern<sup>2</sup>; Laura Santambrogio<sup>1</sup>; <sup>1</sup>Albert Einstein College Medicine, Bronx, NY; <sup>2</sup>University of Massachusetts. Medical School, Worcester, MA
- ThOC pm 3:30 **Incorporation of Ultra-Violet Photodissociation (UVPD) into a Phosphoproteomic Pipeline improves Phosphosite Assignments.**; Kyle L. Fort; Clement M. Potel; Andrey Dyachenko; Albert J.R. Heck; *Utrecht University, Utrecht, Netherlands*
- ThOC pm 3:50 **Photodissociation Study of Hydrogen-Rich and Hydrogen-Deficient Cation Radicals in Tyrosine-Containing Peptides.**; Emilie Viglino; Christopher Shaffer; Frantisek Turecek; *University of Washington, Seattle, Washington*
- ThOC pm 4:10 **Electron Deficient Radical B-Type Ions Undergo Sequence Scrambling and Dissociation by Different Mechanisms than Corresponding b-Ions.**; Declan Williams<sup>1</sup>; Justin Kai-Chi Lau<sup>1, 2</sup>; Stefanie Maedler<sup>1</sup>; Yating Wang<sup>1</sup>; Junfang Zhao<sup>1</sup>; Irine Saminathan<sup>1</sup>; K.W. Michael Siu<sup>1, 2</sup>; Alan C. Hopkinson<sup>1</sup>; <sup>1</sup>York University, Toronto, Canada; <sup>2</sup>University of Windsor, Windsor, Canada

2:30 – 4:30 PM, THURSDAY AFTERNOON  
FORENSIC APPLICATIONS

**Kenyon Evans-Nguyen (University of Tampa) presiding**  
Room 120/127

- ThOD pm 2:30 **Identification of Plant-based Forensic Evidence by Direct Analysis in Real Time Mass Spectrometry (DART-MS), Chemotaxonomic Profiling and Chemometrics;** Ashton D. Lesiak<sup>1</sup>; Justine E. Giffen<sup>1</sup>; Robert B. Cody<sup>2</sup>; A. John Dane<sup>2</sup>; Rabi A. Musah<sup>1</sup>; <sup>1</sup>University at Albany-SUNY, Albany, NY; <sup>2</sup>JEOL USA, Inc., Peabody, MA
- ThOD pm 2:50 **Rapid Analysis of Synthetic Cannabinoids using a Miniature Mass Spectrometer with Ambient Ionization Capability;** Qiang Ma<sup>1,2</sup>; R. Graham Cooks<sup>2</sup>; Zheng Ouyang<sup>2</sup>; <sup>1</sup>Chinese Academy of Inspection and Quarantine, Beijing, China; <sup>2</sup>Purdue University, West Lafayette, IN
- ThOD pm 3:10 **A New Approach in Hair Forensics: Longitudinal Scanning of Drugs of Abuse in Hair using DART-MS;** Wilco F. Duvivier<sup>1</sup>; Teris A. van Beek<sup>1</sup>; Michel W.F. Nielen<sup>1,2</sup>; <sup>1</sup>Wageningen University, Wageningen, The Netherlands; <sup>2</sup>RIKILT-Institute of Food Safety, Wageningen, The Netherlands
- ThOD pm 3:30 **Isobaric Drug Analyses using Hydrogen/Deuterium Exchange and CID;** William D. Hoffmann; Glen P. Jackson; *West Virginia University, Morgantown, WV*
- ThOD pm 3:50 **CSI Sheffield Hallam University: Forensic Analysis of Fingermarks by MALDI MS and the Integration into Currently Employed Fingermark Examination Workflows;** Robert Bradshaw<sup>1</sup>; Neil Denison<sup>2</sup>; Stephen Bleay<sup>3</sup>; Malcolm Clench<sup>1</sup>; Simona Francese<sup>1</sup>; <sup>1</sup>BMRC, Sheffield Hallam University, Sheffield, United Kingdom; <sup>2</sup>Head of Identification Services, Yorkshire and the Humber (YaTH) Regional Policing, United Kingdom; <sup>3</sup>CAST, Home Office UK, St Albans, United Kingdom
- ThOD pm 4:10 **Forensic Serology Testing by Mass Spectrometry;** Heyi Yang<sup>1</sup>; Samantha Monier<sup>2</sup>; Kaylee Hershfeld<sup>1</sup>; Matthew Goldstein<sup>1</sup>; Donald Siegel<sup>1</sup>; <sup>1</sup>Office of Chief Med Exam, New York, NY; <sup>2</sup>Columbia University, New York, NY

2:30 – 4:30 PM, THURSDAY AFTERNOON  
SYNTHETIC POLYMERS

**Wendy Zhong (Merck) presiding**  
Theater

- ThOE pm 2:30 **Characterization of Atmospheric Pressure Polyolefin Pyrolysis Products by Fourier Transform Mass Spectrometry and Ion Mobility – Mass Spectrometry;** Carlos Afonso<sup>1</sup>; Mathilde Farenc<sup>1,2</sup>; Matthias Witt<sup>3</sup>; Kirsten Craven<sup>4</sup>; Caroline Barrère-Mangote<sup>2</sup>; Pierre Giusti<sup>2</sup>; <sup>1</sup>University of Rouen, Mont Saint Aignan, France; <sup>2</sup>TOTAL Refining and Chemicals, Gonfreville l'Orcher, France; <sup>3</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>4</sup>Waters, Manchester, UK
- ThOE pm 2:50 **Analysis of Alkyl Polyglycosides (APGs) using Polarity vs. Shape Sensitive Multidimensional Mass Spectrometry;** Chrys Wesdemiotis; Ahlam Alalwiat; *The University of Akron, Akron, OH*
- ThOE pm 3:10 **Tandem Mass Spectrometry to Read Messages Encoded in Synthetic Copolymers;** Laurence Charles<sup>1</sup>; Jean-François Lutz<sup>2</sup>; <sup>1</sup>Aix-Marseille University, Marseille Cedex 20, France; <sup>2</sup>Institut Charles Sadron, Strasbourg, France
- ThOE pm 3:30 **Iron(III) Catalyzed Branching Reactions of Polymeric Methylene Diphenyl Diisocyanate;** Anthony P. Gies; Zdravko Stefanov; Debashis

Chakraborty; Paul Chauvel; *Dow Chemical Company, Freeport, TX*

- ThOE pm 3:50 **Shining New Light on Nitroxide-Mediated Photopolymerisation by Photodissociation Action Spectroscopy;** David L. Marshall<sup>1</sup>; Jason C Morris<sup>1</sup>; Christopher S Hansen<sup>2</sup>; Adam J Trevitt<sup>2</sup>; Stephen J Blanksby<sup>1</sup>; <sup>1</sup>Queensland University of Technology, Brisbane, Australia; <sup>2</sup>University of Wollongong, Wollongong, Australia
- ThOE pm 4:10 **Application of Matrix-Assisted Ionization-Ion Mobility Spectrometry–Mass Spectrometry to Polymeric Surfaces Directly from Natural Environments;** Casey Foley<sup>1</sup>; Barbara S. Larsen<sup>2</sup>; Sarah Trimpin<sup>1</sup>; <sup>1</sup>Wayne State University, Detroit, MI; <sup>2</sup>The DuPont Company, Wilmington, DE

2:30 – 4:30 PM, THURSDAY AFTERNOON  
CHEMICAL CROSS-LINKING AND COVALENT LABELING  
**Lars Konermann (University of Western Ontario) presiding**  
Room 106

- ThOF pm 2:30 **The Novel Isotopically-Coded Photo-Reactive Homo-Bifunctional Short-Range Crosslinker TATA for Studying Protein Structures.;** Nicholas Brodie<sup>1</sup>; Evgeniy Petrotchenko<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada; <sup>2</sup>Dept. of Biochem. & Microbiol., Univ. of Victoria, Victoria, BC, Canada
- ThOF pm 2:50 **A Highly Optimized Strategy for Dissecting the Architectures of Endogenous Macromolecular Assemblies;** Yi Shi<sup>1</sup>; Riccardo Pellarin<sup>2</sup>; Peter Fridy<sup>1</sup>; Javier Fernandez-Martinez<sup>1</sup>; Mary Thompson<sup>1</sup>; Yinyin Li<sup>1</sup>; Qing Jun Wang<sup>3</sup>; Andrej Sali<sup>2</sup>; Michael Rout<sup>1</sup>; Brian Chait<sup>1</sup>; <sup>1</sup>The Rockefeller University, Nyc, NY; <sup>2</sup>University of California, San Francisco, San Francisco, CA; <sup>3</sup>University of Kentucky, Lexington, KY
- ThOF pm 3:10 **New Tools for Studying Molecular Architecture and Conformational Changes of Large Protein Complexes using Chemical Cross-Linking;** Alexander Leitner<sup>1</sup>; Thomas Walzthoeni<sup>1,2</sup>; Ruedi Aebersold<sup>1,3</sup>; <sup>1</sup>ETH Zurich, Zurich, Switzerland; <sup>2</sup>Gene Center, LMU Munich, Munich, Germany; <sup>3</sup>University of Zurich, Zurich, Switzerland
- ThOF pm 3:30 **A New In Vivo Cross-linking Mass Spectrometry Platform to Define Protein-Protein Interactions in Living Cells;** Kaake Robyn<sup>1</sup>; Xiaorong Wang<sup>1</sup>; Anthony Burke<sup>1</sup>; Clinton Yu<sup>1</sup>; Wynne Kandur<sup>1</sup>; yingying yang<sup>1</sup>; Tonya Second<sup>2</sup>; Jicheng Duan<sup>1</sup>; Athit Kao<sup>1</sup>; Shenheng Guan<sup>3</sup>; Danielle Vellucci<sup>1</sup>; Scott Rychnovsky<sup>1</sup>; Lan Huang<sup>1</sup>; <sup>1</sup>University of California, Irvine, CA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA; <sup>3</sup>University of California, San Francisco, CA
- ThOF pm 3:50 **Hydroxyl Radical Footprinting of Human SOD1 Reveals Solvent Accessibility of the Interior of SOD1  $\beta$ -Barrel;** Yuewei Sheng<sup>1,2</sup>; Puneet Souda<sup>1</sup>; Joan Valentine<sup>1,3</sup>; Julian Whitelegge<sup>1</sup>; <sup>1</sup>University of California, Los Angeles, Los Angeles, CA; <sup>2</sup>Boston University, Boston, MA; <sup>3</sup>Ewha Womans University, Seoul, South Korea
- ThOF pm 4:10 **ETD-Based High Spatial Resolution Hydroxyl Radical Protein Footprinting Reveals an Extended Robo1-Heparin Binding Interface;** Zixuan Li<sup>1</sup>; Heather Moniz<sup>1</sup>; Shuo Wang<sup>1</sup>; Annapoorani Ramiah<sup>1</sup>; Fuming Zhang<sup>2</sup>; Kelley W. Moremen<sup>1</sup>; Robert J. Linhardt<sup>2</sup>; Joshua S. Sharp<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA; <sup>2</sup>Rensselaer Polytechnic Institute, Troy, NY



**2:30 – 4:30 PM, THURSDAY AFTERNOON  
ECOLOGICAL AND HUMAN ENVIRONMENTAL  
CHEMISTRY AND TOXICOLOGY**

**Dana Boyd Barr (Emory University) presiding  
Ballroom 222/224**

- ThOG pm 2:30 **Identification of Unknown Hemoglobin Adducts Based on Adductome LC-MS Data;** Henrik Carlsson; Margareta Törnqvist; *Stockholm University, Stockholm, Sweden*
- ThOG pm 2:50 **Exploring the Mechanism of Neurodegeneration by using an *in vitro* 3D Dopaminergic Cell Model and Metabolomics;** Liang Zhao; Georgina Harris; Lena Smirnova; Thomas Hartung; *Johns Hopkins University, Baltimore, MD*
- ThOG pm 3:10 **LC-MS Method for Simultaneous Detection and Quantification of Common Toxicologically Important Mycotoxins in Human Plasma Samples for Exposure Studies;** Irina Slobodchikova; Cian Monnin; Samiur Rahman; Reajeen Sivakumar; Dajana Vuckovic; *Concordia University, Montreal, Canada*
- ThOG pm 3:30 **Characterization of Petroleum Emerging Environmental Contaminants in Louisiana Salt Marsh Samples Four Years after the Deepwater Horizon Oil Spill;** Steven M. Rowland<sup>1</sup>; Huan Chen<sup>2</sup>; Aixin Hou<sup>3</sup>; Yuri E. Corilo<sup>1, 2</sup>; Qianxin Lin<sup>4</sup>; Jie Lu<sup>1</sup>; Irving A. Mendelssohn<sup>4</sup>; Rui Zhang<sup>3</sup>; Ryan P. Rodgers<sup>2</sup>; Amy M. McKenna<sup>2</sup>; <sup>1</sup>*Future Fuels Institute, FSU, Tallahassee, FL*; <sup>2</sup>*National High Magnetic Field Laboratory, Tallahassee, FL*; <sup>3</sup>*Department of Environmental Sciences, LSU, Baton Rouge, LA*; <sup>4</sup>*Department of Oceanography & Coastal Sciences, LSU, Baton Rouge, LA*
- ThOG pm 3:50 **Compositional Comparison of Weathering Trends for Four Different Oil Spills Determined by Ultrahigh Resolution FT-ICR Mass Spectrometry;** Logan C. Krajewski<sup>1</sup>; Huan Chen<sup>2</sup>; Ryan P. Rodgers<sup>2, 3</sup>; Christopher M. Reddy<sup>4</sup>; Karin T. Lemkau<sup>5</sup>; Christoph Aeppli<sup>6</sup>; Robert F. Swarthout<sup>4</sup>; Alan Marshall<sup>1, 2</sup>; Amy M. McKenna<sup>2</sup>; <sup>1</sup>*Department of Chemistry and Biochemistry, FSU, Tallahassee, FL*; <sup>2</sup>*National High Magnetic Field Laboratory, FSU, Tallahassee, FL*; <sup>3</sup>*Future Fuels Institute, FSU, Tallahassee, FL*; <sup>4</sup>*Woods Hole Oceanographic Institute, Woods Hole, MA*; <sup>5</sup>*University of California, Santa Barbara, CA*; <sup>6</sup>*Bigelow Laboratory for Ocean Sciences, East Boothbay, ME*
- ThOG pm 4:10 **Non-Targeted Analysis to Assess Human Exposure to Semivolatile Organic Contaminants in the Indoor Environment;** Lee Ferguson; Bernadette Vogler; Heather Stapleton; *Duke University, Durham, NC*

**2:30 – 4:30 PM, THURSDAY AFTERNOON  
APPLYING LC-MS TECHNIQUES TO SOLVE CHALLENGING  
DRUG METABOLISM PROBLEMS**

**Natasha Penner (Biogen Idec) presiding  
Ballroom 220/221**

- ThOH pm 2:30 **Changing the Paradigm of Metabolite Analysis in DMPK using UPLC Coupled with High Resolution Mass Spectrometry;** Hongying Gao<sup>1</sup>; Shibing Deng<sup>2</sup>; R. Scott Obach<sup>1</sup>; <sup>1</sup>*Pfizer Inc, Groton, CT*; <sup>2</sup>*Pfizer Inc, San Diego, CA*
- ThOH pm 2:50 **High Resolution LC/MS-based Background Subtraction for Unambiguous Identification of Metabolites of Macrocytic Peptides *in vivo*;** Haiping Zhang; Jennifer X. Qiao; Yue-Zhong Shu; Michael A. Poss; W. Griffith Humphreys; *Bristol-Myers Squibb R&D, Princeton, NJ*

- ThOH pm 3:10 **Characterization of a Selective Androgen Receptor Modulator Drug Candidate and Identification of *in vitro* Generated Metabolites for Sports Drug Testing;** Mario Thevis<sup>1, 2</sup>; Andreas Lagojda<sup>3</sup>; Andreas Thomas<sup>1</sup>; Josef Dib<sup>1</sup>; Annelie Hansson<sup>4</sup>; Mikael Hedeland<sup>4, 5</sup>; Ulf Bondesson<sup>4, 5</sup>; Tina Wigger<sup>6</sup>; Uwe Karst<sup>6</sup>; Wilhelm Schänzer<sup>1</sup>; <sup>1</sup>*German Sport University, Cologne, DE*; <sup>2</sup>*Europ. Monitoring Ctr. for Emerging Doping Agents, Cologne/Bonn, DE*; <sup>3</sup>*BayerCropScience, Monheim, DE*; <sup>4</sup>*Uppsala University, Uppsala, SE*; <sup>5</sup>*Nat'l Veterinary Institute, Uppsala, SE*; <sup>6</sup>*University of Münster, Münster, DE*
- ThOH pm 3:30 **Detection and Quantitation of Insulin Analogues by Differential Mobility Coupled to Mass Spectrometry;** J.C. Yves Leblanc; Brad Schneider; J. Larry Campbell; *SCIEX, Concord, On, Canada*
- ThOH pm 3:50 **Therapeutic Protein Quantitation using Dried Blood Spot Sampling to Support Discovery Stage PK Studies;** Lisa O'Callaghan<sup>1</sup>; Qian Zhang<sup>1</sup>; Daniela Tomazela<sup>2</sup>; Daniel Spellman<sup>1</sup>; Maribel Beaumont<sup>2</sup>; Bao-Jen Shyong<sup>1</sup>; Jacqueline Kenny<sup>1</sup>; Scott Fauty<sup>1</sup>; Kerry Fillgrove<sup>1</sup>; Jane Harrelson<sup>1</sup>; Kevin Bateman<sup>1</sup>; <sup>1</sup>*Merck & Co., West Point, PA*; <sup>2</sup>*Merck & Co., Palo Alto, CA*
- ThOH pm 4:10 **Human *In vivo* Protein Turnover Measurements by Sequential Immunoaffinity and Targeted Mass Spectrometry;** Vahid Farrokhi<sup>1</sup>; Xiaoying Chen<sup>2</sup>; Hendrik Neubert<sup>1</sup>; <sup>1</sup>*Pfizer, PDM-NBE, Andover, MA*; <sup>2</sup>*Pfizer, PDM-NBE, Cambridge, MA*

**PLENARY LECTURE**

**Vicki H. Wysocki (The Ohio State University) presiding  
Hall 5**



**The Evolution of Modern Neurosurgery:  
A History of Trial and Error, Success and  
Failure**

**G. Michael Lemole, Jr.**  
The University of Arizona College of Medicine

**6:30 – 9:00 PM, THURSDAY  
CLOSING EVENT  
CITY MUSEUM  
Ticket is required.**



# MONDAY POSTERS

7:30 – 8:00 am..... Set up all Monday posters  
 10:30 am – 1:00 pm..... Odd-numbered posters present  
 12:00 – 2:30 pm..... Even-numbered posters present  
 7:30 – 8:00 pm..... Remove all Monday posters

MALDI: Sample Preparation.....001-015  
 Ambient Ionization: Application.....016-046  
 Instrumentation: New Developments in Ionization  
 and Sampling.....047-076  
 Instrumentation: New Developments in Mass Analyzers.....077-093  
 LC-MS: Instrumentation and Software.....094-107  
 FAIMS and DMS.....108-125  
 Ion Mobility: Theory .....126-135  
 Ion Mobility: Instrumental.....136-155  
 Imaging MS: Instrumentation.....156-175  
 Imaging MS: Software .....176-184  
 H/D Exchange: Hardware, Software and Methodology .....185-199  
 Top-Down Protein Analysis: Relatively Pure Sample .....200-219  
 Natural Products.....220-246  
 Small Molecules: Quantitative Analysis.....247-276

Drug Discovery/DMPK/ADME .....277-298  
 Diagnostic Clinical Chemistry .....299-332  
 Metabolomics: General.....333-360  
 Metabolomics: Sample Preparation.....361-376  
 Metabolomics: Quantitative Analysis .....377-405  
 Informatics: Metabolomics.....406-418  
 Informatics: Algorithms and Statistical Advances .....419-443  
 Biomarkers: Discovery.....444-466  
 Biomarkers: Quantitative Analysis (Protein) .....467-488  
 Plant-omics.....489-502  
 Proteomics: Tissue .....503-515  
 Proteomics: Quantitative - Label Free Quantification .....516-542  
 Proteomics: Clinical Applications.....543-569  
 Phosphopeptides: Enrichment Methods.....570-580  
 Glycoproteins: Method Development .....581-605  
 Systems Biology: Proteomics .....606-627  
 Systems Biology: Other .....628-641  
 Energy: Hydrocarbon and Petrochemical.....642-666  
 Carbohydrates I.....667-692  
 Special Posters displayed Monday through Thursday.

## MALDI: SAMPLE PREPARATION 001 - 015

- MP 001 **The Analyses of Fluorescently Labeled Biomolecules with Fluorophore-Assisted Laser Desorption/Ionization-Mass Spectrometry (FALDI-MS);** Raymond West; Justin Jacobs; Dragan Isailovic; *University of Toledo, Toledo, OH*
- MP 002 **Peptides Quantification: Improved Performance by the Binary Matrices System for MALDI-TOF-MS;** Milena Luizete; João Luiz Bronzel Junior; Humberto Milagre; *UNESP - Univ Estadual Paulista - Institute of Chem, Araraquara, Brazil*
- MP 003 **Rapid and Simple Fixed-Charge Derivatization of Alcohols for Analysis by MALDI and SALDI Mass Spectrometry;** Roman Borisov; Dmitry Zhilyaev; Nikolai Polovkov; Vladimir Zaikin; *Topchiev Institute of Petrochemical Synthesis, Moscow, Russian Federation*
- MP 004 **Ionic Liquids as Combined CE Additive and MALDI Matrix;** Leila Josefsson; Jessica Bernsteen; Saara Mikkonen; Åsa Emmer; *KTH Royal Institute of Technology, Stockholm, Sweden*
- MP 005 **Simple on-plate PNGase F Digestion Combined with LC/ MALDI-MS for Site-Specific N-glycosylation Analysis;** Ritsuko Yoda; Yusaku Hioki; Takashi Nishikaze; Naoki Kaneko; Hideharu Shichi; Shinichi Iwamoto; Koichi Tanaka; *Shimadzu Corporation, Kyoto, Japan*
- MP 006 **A Bi-Functional Glass Membrane Designed to Interface SDS-PAGE Separations of Proteins with the Detection of Peptides by Mass Spectrometry;** Kenneth Parker; Stephen J. Hattan; Marvin Vestal; *SimulTOF/ VIC Instruments, Sudbury, MA*
- MP 007 **A Fully Automated, Bottom-up Approach for MALDI-TOF MS Based Discovery Workflows;** M. Nazim Boutaghou<sup>1</sup>; David Colquhoun<sup>1</sup>; Kevin W. Meyer<sup>2</sup>; Brian J. Feild<sup>1</sup>; Scott Kuzdzal<sup>1</sup>; <sup>1</sup>*Shimadzu Scientific Instruments, Columbia, MD*; <sup>2</sup>*Perfinity Biosciences, West Lafayette, IN*
- MP 008 **Simple Fabrication of Superhydrophobic AKD Coated MALDI Concentration Plates for Increased Sensitivity;** Johan Jacksén; Joakim Romson; Charlotte Sidenblad; Åsa Emmer; *KTH Royal Institute of Technology, Stockholm, Sweden*
- MP 009 **Optimization of Sample Preparation for Detection of Common Food-borne Pathogens by Matrix-Assisted Laser Desorption Ionization–Time of Flight Mass Spectrometry;** Lay Hoon Seah; Tze Horng Liew; Thye Ngak Mathew Lau; *Singapore, Singapore*
- MP 010 **Evaluation of Microalgae Protein Profile by MALDI-**

- TOFMS with the Increase of TFA Concentration in the sDHB Matrix Solvent;** Lidiane Maria Andrade; Maria Anita Mendes; Claudio Augusto Oller do Nascimento; *Universidade de São Paulo - USP, Sao Paulo, Brazil*
- MP 011 **High-Throughput Screening MALDI-TOF Assays beyond 100,000 Samples per Day;** Sergei Dikler<sup>1</sup>; Scott A. Busby<sup>2</sup>; W. Adam G. Hill<sup>2</sup>; Paul J. Kowalski<sup>1</sup>; Anja Resemann<sup>3</sup>; Detlev Suckau<sup>3</sup>; <sup>1</sup>*Bruker Daltonics Inc., Billerica, MA*; <sup>2</sup>*Novartis Institutes for BioMedical Research Inc., Cambridge, MA*; <sup>3</sup>*Bruker Daltonik GmbH, Bremen, Germany*
- MP 012 **Cyano-phenylenevinylene Oligomer as a Novel Electron Transfer Ionization MALDI Matrix;** Laura Castellanos<sup>1</sup>; Melissa Cely<sup>2</sup>; César A. Sierra<sup>2</sup>; Cristian Blanco-Tirado<sup>1</sup>; Marianny Y. Combariza<sup>1</sup>; <sup>1</sup>*UIS, Bucaramanga, Colombia*; <sup>2</sup>*Universidad Nacional de Colombia, Bogotá, Colombia*
- MP 013 **Rational Design and Efficient Synthesis of cyano-Containing Phenylenevinylene Derivatives as Potential MALDI Matrixes for Electron Transfer Ionization;** Juan Ramirez; *Universidad Industrial de Santander, Floridablanca, Colombia*
- MP 014 **Charged Droplets: Physics and Applications;** Drew Sauter; *Nanoliter, LLC, Henderson, NV*
- MP 015 **Solvent-free Metal Nanoparticle Application and Comparison for Nanoparticle Assisted Laser Desorption Ionization Mass Spectrometry of Plant Metabolites;** Gargey Yagnik<sup>1,2</sup>; Young-Jin Lee<sup>1,2</sup>; <sup>1</sup>*Iowa State University, Ames, Iowa*; <sup>2</sup>*Ames Laboratory-US DOE, Ames, Iowa*

## AMBIENT IONIZATION: APPLICATION 016 - 046

- MP 016 **Investigation of Aqueous Phase Electrochemical Reactions by Desorption Electrospray Ionization Mass Spectrometry;** Mei Lu<sup>1</sup>; Yong Liu<sup>2</sup>; Roy Helmy<sup>2</sup>; Gary Martin<sup>2</sup>; Howard Dewald<sup>1</sup>; Hao Chen<sup>1</sup>; <sup>1</sup>*Ohio University, Athens, OH*; <sup>2</sup>*Merck & Co., Rahway, NJ*
- MP 017 **Breath Analysis Using Direct Analysis in Real Time Mass Spectrometry - A Fun “Food is Chemistry” Student Demonstration;** Curtis Mowry; Adam Pimentel; *Sandia National Laboratories, Albuquerque, NM*
- MP 018 **Reproducibility and Quantitation using Matrix-Assisted Ionization (MAI) Mass Spectrometry;** Shubhashis Chakrabarty<sup>1,2</sup>; Kevin Jooss<sup>2</sup>; Srinivas B. Narayan<sup>3</sup>; Sarah Trimpin<sup>2,4</sup>; <sup>1</sup>*MSTM, LLC., Hockessin, DE*; <sup>2</sup>*Department of Chemistry, Wayne State University, Detroit, MI*; <sup>3</sup>*Detroit Medical Center: Detroit Hospital (DMC), Detroit, MI*; <sup>4</sup>*Cardiovascular Research Institute, Wayne State University*





- School of Medicine, Detroit, MI
- MP 019 **Micro-area Analysis of Tooth Surface Using Surface Desorption Atmospheric Pressure Chemical Ionization Mass Spectrometry;** Qian Li<sup>1</sup>; Haiwei Gu<sup>2</sup>; Jiang Wang<sup>1</sup>; Xiaotun Guo<sup>1</sup>; Eric Handberg<sup>1</sup>; Zhihao Wang<sup>1</sup>; Shuiping Yang<sup>3</sup>; Huanwen Chen<sup>1</sup>; <sup>1</sup>East China Institute of Tech., Nanchang, China; <sup>2</sup>Northwest Metabolomics Research Center, Department, Seattle, WA; <sup>3</sup>East China Institute of Technology, Fuzhou, China
- MP 020 **Atmospheric Pressure Neutral Reionization Mass Spectrometry for Structural Analysis;** Pengyuan Liu; Hao Chen; *Ohio University, Athens, OH*
- MP 021 **The Multifunctional Single-Probe for Single Cell Mass Spectrometry Analysis;** Ning Pan; Zhibo Yang; Wei Rao; Anthony Burgett; Kothapalli Naga Rama; *University of Oklahoma, Norman, OK*
- MP 022 **In vivo Detection of Plant Molecules by Low-Temperature Plasma Mass Spectrometry (LTP-MS);** Sandra Martínez Jarquín; Robert Winkler; *CINVESTAV Unidad Irapuato, Irapuato, Mexico*
- MP 023 **Regulated Generation of Molecular Ions or Protonated Molecules under Atmospheric-Pressure Helium-Plasma-Ionization (HePI) Mass Spectrometric Conditions;** Athula B. Attygalle; Rekha Gangam; Julius Pavlov; *Stevens Institute of Technology, Hoboken, NJ*
- MP 024 **Different Materials Coated Paper Substrates for Paper Spray Mass Spectrometry;** Yajun Zheng<sup>1</sup>; Xiaoling Zhang<sup>1</sup>; Qian Wang<sup>1</sup>; Xinrong Zhang<sup>2</sup>; Zhiping Zhang<sup>1</sup>; <sup>1</sup>Xi'an Shiyou University, Xi'an, China; <sup>2</sup>Tsinghua University, Beijing, China
- MP 025 **Characterization of Large Saturated Hydrocarbons by Automatic Raster Laser-Induced Acoustic Desorption/ Atmospheric Pressure Oxygen Chemical Ionization Mass Spectrometry;** Chunfen Jin<sup>1</sup>; Hanyu Zhu<sup>1</sup>; Alex Dow<sup>1</sup>; Viidanoja Jyrki<sup>2</sup>; Hilkka Kenttämää<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>Neste Oil, Keilaranta, Finland
- MP 026 **Touch Spray Mass Spectrometry with Medical Swabs for Direct Analysis of Bacteria and Drugs in Oral Fluid;** Valentina Pirro<sup>1, 2</sup>; Alan K. Jarmusch<sup>1</sup>; Kevin S. Kerian<sup>1</sup>; Marco Vincenti<sup>2</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Chemistry Department, Purdue University, West Lafayette, IN; <sup>2</sup>Antidoping and Toxicology Center A. Bertinaria, Orbassano, IT
- MP 027 **Microbial Communication through the Air: Analyzing Volatile Bacterial Compounds by Comparative GC-MS and DART-MS Approaches;** Matthew Pavlovich; Violetta Medik; Slava Epstein; Adam Hall; *Northeastern University, Boston, MA*
- MP 028 **Improving Ionization Efficiency of Direct Analysis in Real Time-Mass Spectrometry (DART-MS) by using DC Corona Discharges;** Kanako Sekimoto<sup>1</sup>; Motoshi Sakakura<sup>2</sup>; Hiroshi Hike<sup>2</sup>; Takatomo Kawamukai<sup>2</sup>; Teruhisa Shiota<sup>2</sup>; Mitsuo Takayama<sup>1</sup>; <sup>1</sup>Yokohama City Univ., Yokohama, Japan; <sup>2</sup>AMR Inc., Tokyo, Japan
- MP 029 **Thermal Degradation of  $\beta$ -Carotene and Flavonoids Studied Using Atmospheric Solid Analysis Probe Mass Spectrometry (ASAP-MS);** Xiaoyin Xiao; James Hochrein; Lance Miller; *Sandia National Laboratories, Albuquerque, NM*
- MP 030 **Investigation of Biological Fingerprints Using Atmospheric Solid Analysis Probe Mass Spectrometry (ASAP-MS);** James Hochrein; Xiaoyin Xiao; Lance Miller; Kylea Parchert; Ducle Hayes; *Sandia National Laboratories, Albuquerque, NM*
- MP 031 **A DESI MS Based Screening Method for Phthalates in Consumer Goods;** Sabine Schulz<sup>1</sup>; Sebastian Wagner<sup>1</sup>; Stefanie Gerbig<sup>1</sup>; Herbert Waechter<sup>2</sup>; Detlef Sielaff<sup>3</sup>; Dieter Bohn<sup>4</sup>; Bernhard Spengler<sup>1</sup>; <sup>1</sup>Justus Liebig University Giessen, Giessen, Germany; <sup>2</sup>Bavarian State Laboratory f. Health a. Food safety, Erlangen, Germany; <sup>3</sup>State
- Laboratory of Rhineland-Palatinate, Koblenz, Germany; <sup>4</sup>Hessen State Laboratory, Giessen, Germany
- MP 032 **Single Cell Mass Spectrometry Analysis of Marine Algae: Detection of Creatine;** Mei Sun; Ning Pan; Wawrik Boris; Zhibo Yang; *University of Oklahoma, Norman, OK*
- MP 033 **Comparison of Metabolites from Small Populations of Adherent and Detached Hepatocytes Analyzed by Transmission Geometry LAESI Mass Spectrometry;** Rachelle S. Jacobson; Richard L. Thurston; Akos Vertes; *George Washington University, Washington, DC*
- MP 034 **Profiling Unsaturated Lipids in Tissue Using Reactive Extraction Spray Mass Spectrometry;** Yuan Su; Xiaoxiao Ma; Yu Xia; Zheng Ouyang; *Purdue University, West Lafayette, IN*
- MP 035 **Tandem Mass Spectrum and Collision Cross Section Libraries for High-Throughput Identification of Metabolites in Adherent Hepatocytes by LAESI Mass Spectrometry;** Wei Yuan; Bindesh Shrestha; Akos Vertes; *George Washington University, Washington, DC*
- MP 036 **In situ Ink Analysis from Various Types of Documents by Nanospray Desorption Ionization (nano-DESI) Mass Spectrometry;** Sangwon Cha; Gwangbin Lee; Dongkun Lee; *Hankuk Univ. Foreign Studies, Yongin, South Korea*
- MP 037 **Improved Methods for the Analysis of Human Dried Blood Spot Samples by LESA Mass Spectrometry;** Rian Griffiths; Andrew Creese; Joscelyn Sarsby; Helen Cooper; *University of Birmingham, Birmingham, UK*
- MP 038 **Rapid Evaporative Ionization Mass Spectrometry for Intraoperative Breast Cancer Margin Detection;** Edward R. St. John<sup>1</sup>; Julia Balog<sup>1, 2</sup>; Laura J Muirhead<sup>1</sup>; Abigail VM Speller<sup>1</sup>; Emrys A Jones<sup>2</sup>; Rathi Ramakrishnan<sup>1</sup>; Steven Pringle<sup>2</sup>; Ara Darzi<sup>1</sup>; Daniel R Leff<sup>1</sup>; Zoltan Takats<sup>1</sup>; <sup>1</sup>Imperial College London, London, UK; <sup>2</sup>Waters Corporation, Wilmslow, UK
- MP 039 **Rapid Analysis of Extra Virgin Olive Oil Adulteration with Other Oils with No Sample Preparation using Ambient Ionization Mass Spectrometry;** Avinash Dalmia<sup>1</sup>; Craig M. Whitehouse<sup>2</sup>; <sup>1</sup>PerkinElmer, Shelton, CT; <sup>2</sup>PerkinElmer, Branford, CT
- MP 040 **Graphene Oxide-Assisted Paper Spray For Analysis of Malachite Green;** Fen Shen; Pang-Hung Hsu; *NTOU, New Taipei City, Taiwan (R.O.C.)*
- MP 041 **Increased Disulfide Peptide Sequence Coverage via "Cleavage ON/OFF" Switch during Nano-electrospray;** Guangming Huang; *University of Science and Technology of China/USTC, Hefei, P.R. China*
- MP 042 **Real-time Breath Monitoring of Valproic Acid by Mass Spectrometry with Low Temperature Plasma Ionization Source;** Xiaoxia Gong; Songyue Shi; Gerardo Gamez; *Texas Tech University, Lubbock, TX*
- MP 043 **Reaction Acceleration using Paper Spray Ionization and the Haloform Reaction;** Ryan Bain; Shannon Raab; Christopher Pulliam; R. Graham Cooks; *Purdue University, West Lafayette, IN*
- MP 044 **How to Electro-clean APCI Sources between Injections;** Joseph Di Bussolo; *Thermo Fisher Scientific, West Chester, PA*
- MP 045 **Comparative Depth Resolution of Extractive Analysis Techniques;** Mariam S Elnaggar; *Prosolia, Inc., Indianapolis, IN*
- MP 046 **Depth Profiling of Solid Sample by Dielectric Barrier Discharge Plasma Jet Coupled with Ion Trap Mass Spectrometry;** Songyue Shi; Xiaoxia Gong; Gerardo Gamez; *Texas Tech University, Lubbock, TX*

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- MP 047 **Spectroscopic Characterization of a Windowless, Electron-Beam-Pumped Excimer Lamp (EBEL) in the VUV Spectral Region of 50 – 200 nm;** Hendrik Kersten; Sebastian Klopotoski; Sebastian Winkelmann; Thorsten Benter; *Bergische Universität Wuppertal, Wuppertal, Germany*
- MP 048 **Advancements in Atmospheric-Vacuum Interfaces of Mass Spectrometers with Increased Gas Throughput and Enhanced Sensitivity;** Eloy R. Wouters; Satendra Prasad; Jean-Jacques Dunyach; *Thermo Fisher Scientific, San Jose, CA*
- MP 049 **A Method for Performing In-trap Photoionization in a Miniature Ion Trap Mass Spectrometer;** Corey Stedwell; Daniel Debord; Conor Mullens; Michael Spencer; David Rafferty; *1st Detect Corporation, Webster, TX*
- MP 050 **Direct Real-Time Monitoring and Assessment of Single Leaf Carbon Fixation and Respiration Rates for *Arabidopsis thaliana* by Mass Spectrometry;** Karl K. Weitz<sup>1</sup>; Kim K. Hixson<sup>1</sup>; Mary S. Lipton<sup>1</sup>; Ronald J. Moore<sup>1</sup>; Therese RW. Clauss<sup>1</sup>; Norman G. Lewis<sup>2</sup>; Laurence B. Davin<sup>2</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>*Battelle Pacific Northwest National Laboratories, Richland, WA*; <sup>2</sup>*Washington State University, Pullman, WA*
- MP 051 **New Development of Low Pressure Electrospray Ionization Source;** Rui Wang; Xiaoqiang Zhang; Qiao Jin; Jiaqi Shen; Wenjian Sun; *Shimadzu Research Laboratory (Shanghai) Co. Ltd., Shanghai, China*
- MP 052 **Optimized Conditions for the Analysis of Oligonucleotides by Inductive Based Fluidics Mass Spectrometry;** Robert Ross<sup>1</sup>; Drew Sauter<sup>2</sup>; Patrick A. Limbach<sup>1</sup>; <sup>1</sup>*University of Cincinnati, Cincinnati, OH*; <sup>2</sup>*Nanoliter, LLC, Henderson, NV*
- MP 053 **Development of a Dual-Mode Laminar Flow Ion Source for APPI- and APLI-GC-MS;** Kai Kroll; Walter Wissdorf; Hendrik Kersten; Thorsten Benter; *University of Wuppertal, Wuppertal, Germany*
- MP 054 **Concept Study for a Sensitive and Versatile Chemical Ionization TOF Flight Instrument;** Sascha Albrecht<sup>1</sup>; Armin Afchine<sup>1</sup>; Jochen Barthel<sup>1</sup>; Markus Dick<sup>1</sup>; Heinz Rongen<sup>1</sup>; Fred Stroh<sup>1</sup>; Thorsten Benter<sup>2</sup>; <sup>1</sup>*Forschungszentrum Jülich GmbH, Jülich, Germany*; <sup>2</sup>*University of Wuppertal, Wuppertal, Germany*
- MP 055 **Evaluation of Sonic Spray Ionization Mass Spectrometry for Proteomics Analysis;** Spiros Pergantis; Manos Maurakis; *University of Crete, Heraklion, Greece*
- MP 056 **Investigating Compatibility of Electrospray for LC-MS *in situ* Analysis of Icy Bodies in the Solar System;** Adrian Southard<sup>1</sup>; Stephanie Getty<sup>2</sup>; Jerome Ferrance<sup>3</sup>; Manuel Balvin<sup>2</sup>; Jamie E. Elsila<sup>2</sup>; Ana Mellina Espiritu<sup>2</sup>; Carl Kotecki<sup>2</sup>; Paul Mahaffy<sup>2</sup>; <sup>1</sup>*University Space Research Agency, Greenbelt, Maryland*; <sup>2</sup>*NASA GSFC, Greenbelt, MD*; <sup>3</sup>*J2f engineering, Charlottesville, VA*
- MP 057 **Golf-ball Assisted Electrospray Ionization of Mass Spectrometry for Determination of Trace Amino Acids in Complex Samples;** Yen-Hsien Li; Maw-Rong Lee; *National Chung-Hsing University, Taichung, Taiwan*
- MP 058 **Optimization of a Vacuum Ultraviolet Photoionization source for Gas Chromatography used with a High Resolution Time of Flight Mass Spectrometer;** Lloyd Allen; Viatcheslav Artaev; *LECO Corp., Saint Joseph, MI*
- MP 059 **Direct Sampling, Extraction and Ionization Probe with Screening-Printed Electrode (SPE) Based Paper Spray;** Che-I Liao; Kuo-Lung Ku; *National Chiayi University, Chiayi City, Taiwan*
- MP 060 **A Helium Metastable Seeded Secondary Plasma in the Low MBAR Pressure Regime – Characterization and Evaluation for Mass Spectrometric Applications;** Klaus Brockmann<sup>1</sup>; David Mueller<sup>1</sup>; Jessica Brachthäuser<sup>1</sup>; Hendrik Kersten<sup>1</sup>; Thorsten Benter<sup>1</sup>; Achim von Keudell<sup>2</sup>; Thomas Kuschel<sup>2</sup>; Marc Boeke<sup>2</sup>; Joerg Winter<sup>2</sup>; Michel Aliman<sup>3</sup>; Gennady Fedosenko<sup>3</sup>; Ruediger Reuter<sup>3</sup>; Alexander Laue<sup>3</sup>; Hin Yiu Chung<sup>3</sup>; <sup>1</sup>*University of Wuppertal, Wuppertal, Germany*; <sup>2</sup>*University of Bochum, Bochum, Germany*; <sup>3</sup>*Carl Zeiss SMT, Oberkochen, Germany*
- MP 061 **Micro-plasma Based Pulsed Direct Charge Transfer Stage Coupled to a FT-IT Mass Spectrometer;** Yessica Brachthäuser<sup>1</sup>; David Mueller<sup>1</sup>; Hendrik Kersten<sup>1</sup>; Klaus Brockmann<sup>1</sup>; Thorsten Benter<sup>1</sup>; Michel Aliman<sup>2</sup>; Gennady Fedosenko<sup>2</sup>; Ruediger Reuter<sup>2</sup>; Alexander Laue<sup>2</sup>; Hin Yiu Chung<sup>2</sup>; <sup>1</sup>*University of Wuppertal, Wuppertal, Germany*; <sup>2</sup>*Carl Zeiss SMT, Oberkochen, Germany*
- MP 062 **Coupling a Visible-Wavelength Laser to a MALDI TOF/TOF Mass Spectrometer for the Analyses of Biomolecules;** Raymond West<sup>1</sup>; Eric Findsen<sup>1</sup>; Jens Hoehndorf<sup>2</sup>; Dragan Isailovic<sup>1</sup>; <sup>1</sup>*The University of Toledo, Toledo, OH*; <sup>2</sup>*Bruker Daltonics, Bremen, Germany*
- MP 063 **Proton Transfer Mass Spectrometry (PT-MS) with H<sub>3</sub><sup>+</sup> as Reagent Ions;** David Mueller<sup>1</sup>; Yessica Brachthäuser<sup>1</sup>; Hendrik Kersten<sup>1</sup>; Klaus Brockmann<sup>1</sup>; Thorsten Benter<sup>1</sup>; Michel Aliman<sup>2</sup>; Gennady Fedosenko<sup>2</sup>; Ruediger Reuter<sup>2</sup>; Alexander Laue<sup>2</sup>; Hin Yiu Chung<sup>2</sup>; <sup>1</sup>*University of Wuppertal, Wuppertal, Germany*; <sup>2</sup>*Carl Zeiss SMT, Oberkochen, Germany*
- MP 064 **Investigation of Space Distribution of Elements in Solid Samples using Dielectric Barrier Discharge Probe Coupled with ICP-MS;** Yi Zheng<sup>1</sup>; Zhi Xing<sup>2</sup>; Lipeng Liu<sup>1</sup>; Xiaofeng Yu<sup>1</sup>; Gangqiang Li<sup>1</sup>; <sup>1</sup>*Focused Photonics(Hangzhou),Inc., Hangzhou, China*; <sup>2</sup>*Department of Chemistry, Tsinghua University, Beijing, China*
- MP 065 **A Cryofocuser/Quadrupole Mass Spectrometer Coupled to a Catalysis Unit for Detection of Nitrogen Oxide Catalysis Products;** Weigang Lu<sup>1</sup>; Behrooz Zekavat<sup>1</sup>; Abayomi D. Olaitan<sup>1</sup>; Matthew R. Brantley<sup>1</sup>; Deniz A. Erdogan<sup>2</sup>; Emrah Ozensoy<sup>2</sup>; Touradj Solouki<sup>1</sup>; <sup>1</sup>*Chemistry and Biochemistry Department, Baylor University, Waco, TX*; <sup>2</sup>*Department of Chemistry, Bilkent University, Bilkent, Ankara, Turkey*
- MP 066 **Performance Characterization of a Unique Radio-Frequency Ionization Source;** Abayomi D. Olaitan; Behrooz Zekavat; Matthew R. Brantley; Touradj Solouki; *Department of Chemistry and Biochemistry, Baylor University, Waco, TX*
- MP 067 **Application of ETV-ICP-MS for Determining Trace Teavy Metal Elements in Plants;** Xiaofeng Yu; Ying Li; Lipeng Liu; Jian Li; Yan Liang; Gangqiang Li; *Focused Photonics, Inc., Hangzhou, China*
- MP 068 **Pre-filtering Ions in the Upstream Ion Optics to Improve Instrument Robustness and Dynamic Range;** Graeme Mcalister; Michael W. Senko; *Thermo Fisher Scientific, San Jose, CA*
- MP 069 **nESI and cAPCI Applications of a Controlled Ion Activation Stage (“ion tunnel”);** Marco Thinius; Nele Hartmann; Thorsten Benter; *University of Wuppertal, Wuppertal, Germany*
- MP 070 **Comparison of Selectivity Enhancing Measures in Proton-Transfer-Reaction - Mass Spectrometry;** Christian Lindinger<sup>1</sup>; Alfons Jordan<sup>1</sup>; Lukas Maerk<sup>1</sup>; Jens Herbig<sup>1</sup>; Rene Gutmann<sup>1</sup>; Matteo Lanza<sup>1,2</sup>; Kostiantyn Breiev<sup>1,2</sup>; Eugen Hartungen<sup>1</sup>; Gernot Hanel<sup>1</sup>; Simone Juerschik<sup>1</sup>; Philipp Sulzer<sup>1</sup>; Tilmann D. Maerk<sup>1</sup>; <sup>1</sup>*IONICON Analytik GmbH., Innsbruck, Austria*; <sup>2</sup>*University of Innsbruck, Innsbruck, Austria*
- MP 071 **Operation and Applications of Multimode Inlet Ionization;** Milan Pophristic<sup>1</sup>; Khoa Hoang<sup>2</sup>; Charles N. McEwen<sup>1,2</sup>; <sup>1</sup>*MSTM, LLC., Hockessin, DE*; <sup>2</sup>*University of the Sciences in Philadelphia, Philadelphia, PA*



- MP 072 **SWIFT and MSn for Analysis of Organics in Complex Mars Analog Samples with the MOMA Ion Trap Mass Spectrometer**; [Friso H.W. Van Amerom](#)<sup>1</sup>; Ryan M. Danell<sup>2</sup>; Veronica Pinnick<sup>3</sup>; Xiang Li<sup>3</sup>; Stephanie Getty<sup>3</sup>; Ricardo Arevalo<sup>3</sup>; William Brinckerhoff<sup>3</sup>; Paul Mahaffy<sup>3</sup>; <sup>1</sup>Mini-Mass Consulting, Inc, Hyattsville, MD; <sup>2</sup>Danell Consulting, Inc., Winterville, NC; <sup>3</sup>NASA GSFC, Greenbelt, MD
- MP 073 **UltraAWN-PTR-MS: Ultrasonic Acoustic Wave Nebulization coupled with Proton-Transfer-Reaction Mass Spectrometry**; [Lukas Maerk](#)<sup>1</sup>; Simone Juerschik<sup>1</sup>; David P.A. Kilgour<sup>2</sup>; Benjamin L. Oylar<sup>2</sup>; David R. Goodlett<sup>2</sup>; Alfons Jordan<sup>1</sup>; Christian Lindinger<sup>1</sup>; Jens Herbig<sup>1</sup>; Eugen Hartungen<sup>1</sup>; Gernot Hanel<sup>1</sup>; Philipp Sulzer<sup>1</sup>; Tilmann D. Maerk<sup>1,3</sup>; <sup>1</sup>IONICON Analytik GmbH, Innsbruck, Austria; <sup>2</sup>School of Pharmacy, University of Maryland, Baltimore, MD; <sup>3</sup>University of Innsbruck, Innsbruck, Austria
- MP 074 **Slurry FIA/APCI-MS for Quantitative Real-Time Monitoring of Batch Slurry Reactions: An Alternative Setup**; Zhenqian Zhu<sup>1</sup>; David Cho<sup>2</sup>; John Bartmess<sup>1</sup>; Mary Ellen McNally<sup>3</sup>; Ron Hoffman<sup>3</sup>; Kelsey D. Cook<sup>1</sup>; [Liguo Song](#)<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Tennessee, Knoxville, TN; <sup>2</sup>FBI Laboratory, Quantico, VA; <sup>3</sup>DuPont Crop Protection, Newark, Delaware
- MP 075 **Realistic Modeling of the Ion Funnel using the DSMC Method Accounting for Air Drag and Space Charge**; [Eugene Moskovets](#)<sup>1</sup>; Sergey Gimelshein<sup>2</sup>; Taylor Lilly<sup>3</sup>; <sup>1</sup>MassTech Inc, Columbia, MD; <sup>2</sup>Gimel Inc., Los Gatos, CA; <sup>3</sup>University of Colorado, Colorado Springs, CO
- MP 076 **Native MS using SAWN, a Novel Ionization Source for Waters SYNAPT G2**; [Gloria Yen](#)<sup>1</sup>; Ken Laszlo<sup>2</sup>; Yue Huang<sup>1</sup>; Scott Heron<sup>1</sup>; Matthew Bush<sup>2</sup>; David Goodlett<sup>3</sup>; Erik Nilsson<sup>1</sup>; <sup>1</sup>Deurion LLC, Seattle, WA; <sup>2</sup>University of Washington, Seattle, WA; <sup>3</sup>University of Maryland, Baltimore, MD
- INSTRUMENTATION: NEW DEVELOPMENTS IN MASS ANALYZERS**  
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- MP 077 **Development of High-Precision Digital Waveform Generator to Enable Next Generation Digital Ion Traps and Guides**; [Gregory Brabeck](#); Peter Ta Reilly; Liang Wang; *Washington State University, Pullman, WA*
- MP 078 **Understanding Unperturbed Cyclotron Frequency Generation in FT-ICR MS**; [Konstantin O. Nagornov](#)<sup>1</sup>; Anton N. Kozhinov<sup>1</sup>; Konstantin O. Zhurov<sup>1</sup>; Yury O. Tsybin<sup>1,2</sup>; <sup>1</sup>Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; <sup>2</sup>Spectroswiss Sàrl, Lausanne, Switzerland
- MP 079 **Extended Length Radial Ejection Linear Ion Traps for Higher Ion Capacity and other Modes of Mass Analysis**; [Jae C. Schwartz](#); Philip M Remes; Hans Schweingruber; Eugene Zhuk; Qingyu Song; *Thermo Fisher Scientific, San Jose, CA*
- MP 080 **High-Sensitivity Mass Analysis with a Fourier-Transform Quadrupole Ion Trap Operating with Non-Destructive Ion Detection**; [Michael Schmidt](#)<sup>1</sup>; Albrecht Brockhaus<sup>1</sup>; Stefan Butzmann<sup>1</sup>; Alexander Laue<sup>2</sup>; Michel Aliman<sup>2</sup>; <sup>1</sup>University of Wuppertal, Wuppertal, Germany; <sup>2</sup>Carl Zeiss SMT GmbH, Oberkochen, Germany
- MP 081 **Frequency-Multiple Detection Compatible with Optimized Ion Trap Geometry for Enhanced Fourier Transform Ion Cyclotron Resonance Mass Spectral Resolution**; [Tong Chen](#)<sup>1,2</sup>; Steven C. Beu<sup>3</sup>; Nathan K. Kaiser<sup>1</sup>; Donald F. Smith<sup>1</sup>; Greg T. Blakney<sup>1</sup>; John P. Quinn<sup>1</sup>; Daniel G. McIntosh<sup>1</sup>; Vaughan Williams<sup>1</sup>; Alan G. Marshall<sup>1,2</sup>; Christopher L. Hendrickson<sup>1</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>Florida State University, Tallahassee, FL; <sup>3</sup>S C Beu Consulting, Austin, TX
- MP 082 **Matrix-Assisted Laser Desorption Ionization Distance-of-Flight Mass Spectrometry**; [Steven Ray](#)<sup>1</sup>; Elise Dennis<sup>1</sup>; Christie G. Enke<sup>2</sup>; David W. Koppenaal<sup>3</sup>; Charles Barinaga<sup>3</sup>; Gary Hieftje<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN; <sup>2</sup>University of New Mexico, Placitas, NM; <sup>3</sup>Pacific NW Nat'l Laboratory, Richland, WA
- MP 083 **Theoretical Study of a Toroidal Ion Trap Mass Analyzer with Triangular Electrode**; [Haiyang Yang](#); Lei Yue; Chongsheng Xu; *Shanghai, China*
- MP 084 **Duty Cycle Based Manipulation of Ion Motion in Digitally-Operated Ion Traps for Improved Mass Analysis**; [Peter T A Reilly](#)<sup>1</sup>; Katherine Donahoe<sup>1</sup>; Shimin Tan<sup>2</sup>; James Riggelman<sup>2</sup>; <sup>1</sup>Washington State University, Pullman, WA; <sup>2</sup>Pullman High School, Pullman, WA
- MP 085 **A Compact, Versatile and Bipolar Time-of-Flight Mass Spectrometer Tailored for Proton-Transfer-Reaction Mass Spectrometry**; [Alfons Jordan](#)<sup>1</sup>; Lukas Maerk<sup>1</sup>; Christian Lindinger<sup>1</sup>; Stefan Haidacher<sup>1</sup>; Paul Mutschlechner<sup>1</sup>; Stefan Feil<sup>1</sup>; Ralf Schottkowsky<sup>1</sup>; Jens Herbig<sup>1</sup>; Eugen Hartungen<sup>1</sup>; Gernot Hanel<sup>1</sup>; Simone Juerschik<sup>1</sup>; Philipp Sulzer<sup>1</sup>; Tilmann Maerk<sup>1,2</sup>; <sup>1</sup>IONICON Analytik GmbH, Innsbruck, Austria; <sup>2</sup>University of Innsbruck, Innsbruck, Austria
- MP 086 **Nonlinear Corrections of the Fields of Electrostatic FT Mass-Analyzers Aimed at Increasing Their Dynamic Range**; [Gleb Vladimirov](#)<sup>1,2</sup>; Pavel Ryumin<sup>5</sup>; Oleg Kharybin<sup>2,3</sup>; Victor Zgoda<sup>3</sup>; Eugene Nikolaev<sup>2,4</sup>; <sup>1</sup>Skolkovo Institute of Science and Technology, Skolkovo, Moscow Oblast, Russia; <sup>2</sup>Institute for Energy Problems of Chemical Physics, Moscow, Russia; <sup>3</sup>V.N. Orekhovich Institute of Biomedical Chemistry, Moscow, Russia; <sup>4</sup>Moscow Institute of Physics and Technology, Dolgoprudny, Moscow Oblast, Russia; <sup>5</sup>University of Reading, Reading, UK
- MP 087 **A Novel Instrumental Strategy for Parallel Reaction Monitoring of Intact Proteins with an Orbitrap**; Mikhail Belov<sup>1,2</sup>; [Dmitry Grinfeld](#)<sup>2</sup>; Philip Compton<sup>3</sup>; Neil Kelleher<sup>3</sup>; Alexander Makarov<sup>2</sup>; <sup>1</sup>Spectrograph LLC, Kennewick, WA; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>3</sup>Northwestern University, Evanston, IL
- MP 088 **Super-resolution Signal Processing Leverages Multiplexed Quantitative Proteomics**; [Anton N. Kozhinov](#)<sup>1</sup>; Martin Wuehr<sup>2</sup>; John Corthésy<sup>3</sup>; Konstantin O. Nagornov<sup>1</sup>; Kristina Srzentic<sup>1</sup>; Loïc Dayon<sup>3</sup>; Martin Kussmann<sup>3</sup>; Steven P. Gygi<sup>2</sup>; Yury O. Tsybin<sup>1,4</sup>; <sup>1</sup>Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; <sup>2</sup>Harvard Medical School, Boston, MA; <sup>3</sup>Nestlé Institute of Health Sciences, Lausanne, Switzerland; <sup>4</sup>Spectroswiss Sàrl, Lausanne, Switzerland
- MP 089 **An Improved Linear Ion Trap Mass Analyzer built with Polyline-shaped Electrodes**; Chongsheng Xu; *Fudan University, Shanghai, China*
- MP 090 **Juggling Multi-Parameter Optimizations of the Miniature Cylindrical Ion Trap**; [Daniel DeBord](#); Conor Mullens; Michael Spencer; David Rafferty; *1st Detect Corporation, Webster, TX*
- MP 091 **Developing a 2D Ion Trap for the Analysis of Low Charge Intact Proteins**; [Katherine Donahoe](#); Peter Ta Reilly; *Washington State University, Pullman, WA*
- MP 092 **A High Resolution Multi-turn TOF Mass Analyzer**; [Vyacheslav Shchepunov](#); Michael Rignall; Roger Giles; Hiroaki Nakanishi; *Shimadzu Research Laboratory (Europe) Ltd., Manchester, UK*
- MP 093 **Direct Current Enhanced Ion Excitation and Collision-Induced Dissociation in Digital Ion Trap Mass Spectrometer**; [Fuxing Xu](#)<sup>1</sup>; Qiankun Dang<sup>1</sup>; Xinhua Dai<sup>2</sup>; Xiang Fang<sup>2</sup>; Li Ding<sup>1</sup>; Yuanyuan Wang<sup>1</sup>; ChuanFan Ding<sup>1</sup>; <sup>1</sup>Fudan University, Shanghai, China; <sup>2</sup>National Institute of Metrology, Beijing, China

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- MP 094 **Liquid Chromatography Direct Electron Ionization Mass Spectrometry for the Analysis of Polycyclic Aromatic Hydrocarbons;** Mitchell Helling; Franco Basile; *University of Wyoming, Laramie, WY*
- MP 095 **Advanced Electron Ionization LC-MS with Supersonic Molecular Beams - Advantages and Benefits;** Svetlana Tsizin; Boaz Seemann; Alexander Fialkov; Aviv Amirav; *Tel Aviv University, Tel Aviv, Israel*
- MP 096 **Dry Ion localization and locomotion (DRILL) Interface using Vortex Flow Hydrodynamics for Enhanced Sensitivity of Electrospray Ionization Mass Spectrometry;** Willem Schuttler; Andrei Fedorov; Peter Kottke; *Georgia Institute of Technology, Atlanta, GA*
- MP 097 **Time-alignment of Quantitative Isotope Dilution MRM Traces - Integration and Review of 10,000 Aligned Traces in 10 minutes;** Adrian R Woolfitt; Maria Solano; Katie Isbell; Anne Boyer; John Barr; *CDC, Atlanta, GA*
- MP 098 **Direct Analysis of 10 Antipsychotics in Serum by the Online System Integrating SPE with UHPLC-MS/MS;** Qisheng Zhong; Xiongqiong Qiu; Linlin shen; Jinting Yao; Song Zhan; Taohong Huang; Shin-ichi Kawano; Yuki Hashi; *Shimadzu Global COE, Shimadzu (China) Co., Ltd., Guangzhou, China*
- MP 099 **Direct-ESI UHPLC-MSMS as a New Tool for the Analysis of Sterols in Pharmaceuticals and Complex Biological Matrices;** Achille Cappiello<sup>1</sup>; Veronica Termopoli<sup>1</sup>; Famigliini Giorgio<sup>1</sup>; Pierangela Palma<sup>1</sup>; Silvia Spinozzi<sup>2</sup>; Cecilia Camborata<sup>2</sup>; Aldo Roda<sup>2</sup>; <sup>1</sup>*University of Urbino, Urbino, Italy*; <sup>2</sup>*University of Bologna, Bologna, Italy*
- MP 100 **Identification of Biologic Catabolites Using a Q-ToF and Software-Driven Workflow;** Yilin Feng<sup>1</sup>; Panos Hatsis<sup>1</sup>; Suma Ramagiri<sup>2</sup>; Eva Duchoslav<sup>2</sup>; Lyle Burton<sup>2</sup>; Jimmy Flarakos<sup>1</sup>; <sup>1</sup>*Novartis Institutes for Biomedical Research, East Hanover, NJ*; <sup>2</sup>*AB SCIEX, Concord, ON*
- MP 101 **The Sliding Window Algorithm for the Analysis of LC/MS Intact Protein Data;** Paul Gazis; *Thermo Fisher, San Jose, CA*
- MP 102 **An Innovative Software Solution for Multi-Vendor Open Access Data;** David Hardy<sup>1</sup>; Vitaly Lashin<sup>2</sup>; Patrick Wheeler<sup>3</sup>; Pranas Japertas<sup>4</sup>; <sup>1</sup>*ACD/Labs, Bracknell, UK*; <sup>2</sup>*ACD/Labs, Toronto, Canada*; <sup>3</sup>*ACD/Labs, San Diego, CA*; <sup>4</sup>*ACD/Labs, Vilnius, Lithuania*
- MP 103 **Separation and Quantitation of Multicomponent Solutions Using a Novel UHPLC-MSMS System;** Jonathan McNally<sup>1</sup>; Keeley Murphy<sup>1</sup>; Jonathan L. Josephs<sup>1</sup>; Mary Blackburn<sup>1</sup>; Remco Swart<sup>2</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*Thermo Fisher Scientific, Germering, Germany*
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- MP 105 **Open Access Software For Recombinant Protein Characterization;** Edmond Neo; Robert Yang; Kenneth McGreevy; Robin Scheiderer; Maithilee Samant; Ning Tang; Patrick D. Perkins; *Agilent Technologies, Santa Clara, CA*
- MP 106 **A Method for Improved LC-MS/MS Peak Integration by using Multiple Traces and Peak Modeling;** Richard King<sup>1</sup>; John Gibbons<sup>2</sup>; Lyle Burton<sup>2</sup>; Gordana Ivosev<sup>2</sup>; <sup>1</sup>*PharmaCadence Analytical Services, LLC, Hatfield, PA*; <sup>2</sup>*SCIEX, Concord, Ontario, Canada*
- MP 107 **Getting the Most Out of Your Mass Spectrometer – Multiplexing LC/MS Assays for High Throughput;** Todd Lusk; James Lauzun; Daniel Mulvana; *Quintiles, Ithaca, NY*

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- MP 110 **Selextion™ Mobility Separation of Leukotriene Isomers;** Cyrus Papan<sup>1</sup>; Sebastian Fabritz<sup>1</sup>; Martin Giera<sup>2</sup>; <sup>1</sup>*Sciex, Darmstadt, Germany*; <sup>2</sup>*Leids Universitair Medisch Centrum, Leiden, Netherlands*
- MP 111 **Optimization of FAIMS Electrodes for Small Molecule Analysis at High Liquid Flow Rates;** Randy W. Purves<sup>1</sup>; Michael Belford<sup>2</sup>; Satendra Prasad<sup>2</sup>; Jean Jacques Dunyach<sup>2</sup>; Albert Vandenberg<sup>1</sup>; <sup>1</sup>*University of Saskatchewan, Saskatoon, Canada*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*
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- MP 113 **Differential Mobility Separation Prior to Data-Dependent and Data-Independent MS Analysis of Complex Human Proteomics Samples;** Sabine Amon<sup>1</sup>; Stephen A. Tate<sup>2</sup>; Ruedi Aebersold<sup>1, 3</sup>; <sup>1</sup>*Institute of Molecular Systems Biology, ETH Zurich, Zurich, Switzerland*; <sup>2</sup>*AB Sciex, Concord, ON, Canada*; <sup>3</sup>*Faculty of Science, University of Zurich, Zurich, Switzerland*
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- MP 119 **Differential Mobility Spectrometry Analysis of Glycans and Glycopeptides;** Chang Liu; J.C. Yves Leblanc; J. Larry Campbell; Tim L. Hoffman; *SCIEX, Concord, ON, Canada*
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- MP 122 **Method Development for Cirrhosis Biomarkers in Simulated Breath using Various Ionization Techniques Combined with MS and FAIMS;** [Robin H.J. Kemperman](#); Michael T. Costanzo; Christopher R. Beekman; Christopher D. Chouinard; Richard A. Yost; *University of Florida, Gainesville, FL*
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- MP 164 **Matrix-Free Atmospheric Pressure Ultraviolet-Laser Ablation Electrospray Ionization Mass Spectrometry for Plant Material Imaging**; Katherine-Jo Galayda<sup>1,2</sup>; Patrick McVey<sup>1</sup>; Stanely Bajic<sup>2</sup>; R.S. Houk<sup>1</sup>; <sup>1</sup>Iowa State University, Ames, IA; <sup>2</sup>Ames Laboratory, Ames, IA
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- MP 167 **An Enhanced Droplet-Based Liquid Microjunction Surface Sampling System Coupled with HPLC-ESI-MS/MS for Spatially Resolved Analysis**; Vilmos Kertesz<sup>1</sup>; Taylor M. Weiskittel<sup>2</sup>; Gary J. Van Berkel<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>ORISE HERE Intern, University of Tennessee, Knoxville, TN
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- MP 169 **Patterning Matrices to Assess Spatial Resolution in MALDI Imaging Mass Spectrometry in the Range of 10- 100 um**; Faizan Zubair; Paul Kempler; Paul Laibinis; Richard Caprioli; *Vanderbilt University, Nashville, TN*
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- MP 175 **MS-FRAP or MALDI Imaging Setups With Programmable Laser Sources: A New Way to the Diffusion, Molecular Mobility and Binding Measurements;** A. JablOKow<sup>1</sup>; O. Gradow<sup>2</sup>; <sup>1</sup>National Research Medical University, Moscow, RF; <sup>2</sup>Institute of Energy Problems of Chemical Physics, Moscow, RF
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- MP 176 **Multivariate Analysis of Ion-Mobility MALDI MSI Data: Mapping Location, Mass, Charge and Shape;** Alan Race; Josephine Bunch; *National Physical Laboratory, Teddington, UK*
- MP 177 **msIQuant Software – Fast Access, Visualization and Analysis of Very Large MSI Datasets without Data Reduction;** Patrik Kallback; Mohammadreza Shariatgorji; Anna Nilsson; Per E. Andren; *Uppsala University, Uppsala, Sweden*
- MP 178 **Exploring Head and Neck Cancer by MALDI FT-ICR Mass Spectrometric Imaging;** Lukas Krasny<sup>1</sup>; Franziska Hoffmann<sup>2</sup>; Günther Ernst<sup>2</sup>; Jan Hendrik Kobarg<sup>3</sup>; Dennis Trede<sup>3, 4</sup>; Michael Becker<sup>5</sup>; Theodore Alexandrov<sup>4, 6</sup>; Vladimir Havlicek<sup>1</sup>; Orlando Guntinas-Lichius<sup>7</sup>; Ferdinand von Eggeling<sup>2, 7</sup>; Anna C. Crecelius<sup>8, 9</sup>; <sup>1</sup>Institute of Microbiology, v.v.i., Prague, Czech Republic; <sup>2</sup>Institute of Physical Chemistry, Friedrich Schiller University Jena, Germany; <sup>3</sup>Steinbeis Innovation Center SCiLS Research, Bremen, Germany; <sup>4</sup>SCiLS GmbH, Bremen, Germany; <sup>5</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>6</sup>European Molecular Biology Laboratory, Heidelberg, Germany; <sup>7</sup>Department of Otorhinolaryngology, Jena University Hospital, Germany; <sup>8</sup>Jena Center for Soft Matter (JCSM), Friedrich Schiller University Jena, Germany; <sup>9</sup>Laboratory of Organic and Macromolecular Chemistry, Friedrich Schiller University Jena, Germany
- MP 179 **Quantification and Fusion of Mass Spectrometry Imaging Data with MSiReader;** Kenneth Garrard; Mark Bokhart; Milad Nazari; Elias Rosen; David Muddiman; *North Carolina State University, Raleigh, NC*
- MP 180 **Absorption Mode Analysis of FT-ICR Imaging Data Improves Peak Resolution in a Bordetella pertussis Infection Model;** Alison Scott; David Kilgour; Ciaran Skeery; Nicholas Carbonetti; Robert Ernst; David Goodlett; *University of Maryland, Baltimore, MD*
- MP 181 **Development of Methods for Evaluation of Spatial Clustering in Mass Spectrometry Imaging (MSI);** Alexander Dexter<sup>1, 2</sup>; Helen Cooper<sup>1</sup>; Iain Styles<sup>1</sup>; Josephine Bunch<sup>2</sup>; <sup>1</sup>University of Birmingham, Birmingham, UK; <sup>2</sup>The National Physical Laboratory, Teddington, UK
- MP 182 **Inter-Day Normalization of Multi-Imaging Mass Spectrometry Data for Biomarker Discovery;** Fabien Pamelard<sup>1</sup>; Sebastien Dumas<sup>2</sup>; Gregory Hamm<sup>1</sup>; David Bonnel<sup>1</sup>; Gael Picard-de-Muller<sup>1</sup>; Kevin Lorgouilloux<sup>1</sup>; Sylvia Cohen-Kaminsky<sup>2</sup>; Jonathan Stauber<sup>1</sup>; <sup>1</sup>ImaBiotech, MS Imaging Dept., Loos, France; <sup>2</sup>INSERM UMR-S 999, Univ. Paris-Sud, Le Plessis Robinson, France
- MP 183 **Multi-modal Image Fusion for Enhanced On-tissue Molecular Identification;** Raf Van de Plas<sup>1, 2</sup>; Jeffrey Spraggins<sup>2</sup>; Junhai Yang<sup>2</sup>; Richard M. Caprioli<sup>2</sup>; <sup>1</sup>Delft University of Technology, Delft, Netherlands; <sup>2</sup>Vanderbilt University, Nashville, TN
- MP 184 **An Open Cloud-Computing Platform for Efficient Access to Big Data from High-Resolution Imaging Mass Spectrometry;** Sergey Nikolenko<sup>1, 2</sup>; Andrew Palmer<sup>3</sup>; Theodore Alexandrov<sup>3, 4</sup>; <sup>1</sup>National Research University Higher School of Econ, St. Petersburg, Russia; <sup>2</sup>Steklov Institute of Mathematics at St. Petersburg, St. Petersburg, Russia; <sup>3</sup>European Molecular Biology Laboratory, Heidelberg, Germany; <sup>4</sup>SCiLS GmbH, Bremen, Germany
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- MP 186 **Online Strong Cation Exchange and Reversed-Phase Extraction Method for Hydrogen Exchange Mass Spectrometry of Samples Containing Macromolecular Crowding Agents;** Farai Rusinga; *University of Kansas, Lawrence, KS*
- MP 187 **Hydrogen Deuterium Exchange – Mass Spectrometry (HDX-MS) of the Fab Fragment of the NIST-Monoclonal Antibody;** Jeffrey W. Hudgens<sup>1, 2</sup>; Elyssia Gallagher<sup>1, 2</sup>; Ioannis Karageorgos<sup>1, 2</sup>; <sup>1</sup>National Institute of Standards and Technology, Rockville, MD; <sup>2</sup>Institute for Bioscience & Biotechnology Research, Rockville, MD
- MP 188 **The Nuances in Pressurized On-Line Pepsin Digestions of mAbs and the Implications for Hydrogen/Deuterium Exchange Mass Spectrometry;** Jing Fang; Ying-Qing Yu; Asish Chakraborty; Keith Fadgen; Michael Eggertson; Weibin Chen; *Waters Corporation, Milford, MA*
- MP 189 **Multivariate Statistical Tool for Large Scale HDX Drug Screening;** Joey Sheff; *University of Calgary, Calgary, Canada*
- MP 190 **Tuning Peptide Scoring Functions in HX-MS<sup>2</sup> to Support Rapid Data Validation;** Kyle Burns; Vladimir Sarpe; David Schriemer; *University of Calgary, Calgary, Canada*
- MP 191 **Automating Analysis of the SOD1 Protein by H/D Exchange Mass Spectrometry using Single Droplet Digital Microfluidics;** Huijiang John Ding; Joseph Capri; Julian Whitelegge; *University of California LA, Los Angeles, CA*
- MP 192 **A New in-ESI Source Hydrogen/Deuterium Exchange Method and Its Application for Proteomics, Glycomics and Petroleomics;** Yury Kostyukovich<sup>4</sup>; Alexey Kononikhin<sup>2</sup>; Igor Popov<sup>3</sup>; Eugene Nikolaev<sup>1</sup>; <sup>1</sup>Institute for Energy Problems of Chemical Physics, Moscow, Russia; <sup>2</sup>Institute for Energy Problems of Chemical Physics, Moscow, Russian Federation; <sup>3</sup>IBCP RAS, Moscow, Russian Federation; <sup>4</sup>Skolkovo Institute of Science and Technology, Moscow Region, Skolkovo,
- MP 193 **A Statistical Approach to the Deconvolution of Bimodal H/D exchange Data;** Miklos Guttman; Kelly Lee; *University of Washington, Seattle, WA*
- MP 194 **A Data-Driven Approach to Filtering HDX-MS Datasets;** Bruce Pascal<sup>2</sup>; Scott Novick<sup>2</sup>; Devrishi Goswami<sup>2</sup>; Manuel Molina-Martin<sup>3</sup>; Alfonso Espada<sup>3</sup>; Jeffrey Dodge<sup>1</sup>; Michael Chalmers<sup>1</sup>; Pat Griffin<sup>2</sup>; <sup>1</sup>Eli Lilly and Company, Indianapolis, IN; <sup>2</sup>The Scripps Research Institute, Scripps Florida, Jupiter, FL; <sup>3</sup>Lilly S.A., Alcobendas, Spain
- MP 195 **Analyzing Nucleosome Dynamics using Hydrogen-Deuterium Exchange Coupled to Top-Down Mass Spectrometry;** Kelly Karch; Benjamin Garcia; *University of Pennsylvania, Philadelphia, PA*



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- MP 197 **Facile Measurement of Global Exchange Kinetics for PEGylated Proteins;** Cedric Bobst<sup>1</sup>; Damian Houde<sup>2</sup>; George Bou-Assaf<sup>2</sup>; Andrew Weiskopf<sup>2</sup>; Igor Kaltashov<sup>1</sup>; <sup>1</sup>*University of Massachusetts, Amherst, MA*; <sup>2</sup>*Biogen IDEC, Cambridge, MA*
- MP 198 **Optimization of a Fully Automated Hydrogen/Deuterium Exchange Mass Spectrometry Platform to Probe Protein Conformation/Conformation Dynamics;** Terry Zhang<sup>1</sup>; Kai Scheffler<sup>2</sup>; Jonathan Josephs<sup>1</sup>; <sup>1</sup>*ThermoFisher, San Jose, CA*; <sup>2</sup>*ThermoFisher, Dreieich, Germany*
- MP 199 **Ion Mobility Spectrometry-Hydrogen Deuterium Exchange Mass Spectrometry of Anions: Complementing Cation Studies;** Mahdiar Khakinejad<sup>1</sup>; Stephen Valentine<sup>2</sup>; <sup>1</sup>*Morgantown, WV*; <sup>2</sup>*West Virginia University, Morgantown, WV*
- TOP-DOWN PROTEIN ANALYSIS PROTEIN ANALYSIS: RELATIVELY PURE SAMPLE**  
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- MP 200 **Top-Down Electron-Capture Dissociation of Proteins in a QTOF Mass Spectrometer;** Douglas F. Barofsky; Valery G. Voinov; Yury V Vasil'ev; Joseph S. Beckman; *Oregon State University, Corvallis, OR*
- MP 201 **A Top-Down Mass Spectrometry Assay for Effective Protein Denaturation Based Upon Dimethylation of Primary Amines;** Joseph Capri; Whitaker Cohn; Sara Bassilian; Kym Faull; Julian Whitelegge; *University of California LA, Los Angeles, CA*
- MP 202 **Sequence Confirmation of the Protein Therapeutic Granulocyte-Colony Stimulating Factor by Top Down MS/MS and MS3;** Michaela Levy; Ashley Gucinski; Michael Boyne; *U.S. FDA, Saint Louis, MO*
- MP 203 **Deciphering Putative Histone Modification Codes Involved in Control of Gene Expression in Fungi with Top-Down Mass Spectrometry;** Mowei Zhou<sup>1</sup>; Rosalie Chu<sup>1</sup>; David Stenoien<sup>1</sup>; Si Wu<sup>2</sup>; Lanelle Connolly<sup>3</sup>; Jonathan Galazaka<sup>3</sup>; Michael Freitag<sup>3</sup>; Ljiljana Paša-Tolić<sup>1</sup>; <sup>1</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>2</sup>*University of Oklahoma, Norman, OK*; <sup>3</sup>*Oregon State University, Corvallis, OR*
- MP 204 **Conformational Footprinting of Proteins using a Combination of Native Top-Down Electron Transfer Dissociation and Ion Mobility Mass Spectrometry;** Albert Konijnenberg<sup>1</sup>; Frank Sobott<sup>1,2</sup>; <sup>1</sup>*Universiteit Antwerpen, Antwerp, België*; <sup>2</sup>*Center for Proteomics (CFP-CeProMa), Antwerp, Belgium*
- MP 205 **Improving Protein Sequence Coverage and Identification of Oxidation Sites via Top/Middle-Down Fragmentation and Ion-mobility Time-of-flight Mass Spectrometry;** Stephane Houel<sup>1</sup>; Catalin Doneanu<sup>1</sup>; Asish Chakraborty<sup>1</sup>; Andrew Tudor<sup>2</sup>; Nick Tomczyk<sup>2</sup>; Martin Palmer<sup>2</sup>; Weibin Chen<sup>1</sup>; <sup>1</sup>*Waters Corp, Milford, MA*; <sup>2</sup>*Waters MS Technologies, Wilmslow, UK*
- MP 206 **Top-Down FT-ICR Mass Spectrometry for Determination of Site-Specific Protein Disulfide Bond Redox Potentials;** Xiaoyan Guan<sup>1</sup>; Nicolas L. Young<sup>2</sup>; Alan G. Marshall<sup>2</sup>; <sup>1</sup>*National High Magnetic Field Lab, Tallahassee, FL*; <sup>2</sup>*NHMFL / FSU, Tallahassee, FL*
- MP 207 **Top-down MALDI In-Source Decay FTICR-MS of Isotopically Resolved Proteins at an Extended Mass Range;** Simone Nicolardi; Linda Switzar; André M. Deelder; Magnus Palmblad; Yuri E.M. van der Burgt; *Leiden University Medical Center (LUMC), Leiden, The Netherlands*
- MP 208 **Impact of Charge State and Charge Sites on Top-Down Characterization of Proteins using 193 nm Ultraviolet Photodissociation Mass Spectrometry;** Sylvester Greer; Jennifer Brodbelt; *The University of Texas, Austin, Texas*
- MP 209 **Two-dimensional IRMPD/ECD FT-ICR Mass Spectrometry of Calmodulin: A Top-Down and Bottom-Up Approach;** Federico Floris<sup>1</sup>; Maria Van Agthoven<sup>1</sup>; Lionel Chiron<sup>2</sup>; Christopher Wootton<sup>1</sup>; Mark Barrow<sup>1</sup>; Peter B. O'connor<sup>1</sup>; <sup>1</sup>*University of Warwick, Coventry, UK*; <sup>2</sup>*CASC4DE, Illkirch-Graffenstaden, France*
- MP 210 **Mapping Electrostatic Interactions in Protein Ions using Electron Transfer Dissociation;** Zhe Zhang; Richard Vachet; *University of Massachusetts, Amherst, MA*
- MP 211 **In situ Unwrapping of Overlapping Isotopic Envelopes in Protein Tandem Mass Spectra with DREAM in ProteinGoggle;** Zhixin Tian; Kaijie Xiao; Fan Yu; Houqin Fang; Bingbing Xue; Yan Liu; *Department of Chemistry, Tongji University, Shanghai, China*
- MP 212 **Development of a Diagnostic Technique for the Identification of Hemoglobin Variants;** Matthew Edgeworth<sup>1</sup>; Jeff Brown<sup>2</sup>; Jonathan Williams<sup>2</sup>; James Scrivens<sup>1</sup>; <sup>1</sup>*Univ of Warwick, Coventry, UK*; <sup>2</sup>*Waters, Wilmslow, UK*
- MP 213 **Analysis of Intact p53 Protein by Top-Down Mass Spectrometry;** Caroline J. DeHart<sup>1</sup>; Owen S. Skinner<sup>1</sup>; Philip D. Compton<sup>1</sup>; Paul M. Thomas<sup>1</sup>; Galit Lahav<sup>2</sup>; Jeremy Gunawardena<sup>2</sup>; Neil L. Kelleher<sup>1</sup>; <sup>1</sup>*Northwestern University, Evanston, IL*; <sup>2</sup>*Harvard Medical School, Boston, MA*
- MP 214 **Characterization of Histones H2A/H2B in Human Pluripotent Stem Cells;** Xibe Dang<sup>1</sup>; Amar Singh<sup>2</sup>; Stephen Dalton<sup>2</sup>; Alan G. Marshall<sup>1,3</sup>; Nicolas L. Young<sup>3</sup>; <sup>1</sup>*Florida State University, Tallahassee, FL*; <sup>2</sup>*University of Georgia, Athens, GA*; <sup>3</sup>*National High Magnetic Field Laboratory, Tallahassee, FL*
- MP 215 **Comprehensive Characterization of AMP-activated Protein Kinase Catalytic Domain Using Top-Down Mass Spectrometry;** Deyang Yu; Ying Peng; Serife Ayaz-Guner; Ying Ge; *UW-Madison, Madison, WI*
- MP 216 **Top-down (phospho-)Proteiform Characterization by EThcD and UVPD on a Orbitrap Fusion or Exactive EMR;** Andrea Brunner<sup>1</sup>; Philip Lössl<sup>1</sup>; Andrey Dyachenko<sup>1</sup>; Romain Huguet<sup>2</sup>; Christopher Mullen<sup>2</sup>; Vlad Zabrouskov<sup>2</sup>; Alexander Makarov<sup>3</sup>; Albert Heck<sup>1</sup>; A.F. Maarten Altelaar<sup>1</sup>; <sup>1</sup>*Utrecht University, Utrecht, Netherlands*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>3</sup>*Thermo Fisher Scientific, Bremen, Germany*
- MP 217 **Characterization of a Monoclonal Antibody (mAb) using Multiple Fragmentation Techniques and Novel FT Data Processing Software;** Bao Quoc Tran; Shivangi Awasthi; Tao Liang; Modh M. Khan; David Kilgour; David Goodlett; Young Ah Goo; *University of Maryland Baltimore, Baltimore, MD*
- MP 218 **Hemoglobin Variant Analysis by MALDI-MS on TOF/TOF MS and FT-ICR MS Platforms;** Roger Theberge<sup>1</sup>; David H. K. Chui<sup>1</sup>; Carolyn Hoppe<sup>2</sup>; Cheng Lin<sup>1</sup>; Catherine E. Costello<sup>1</sup>; Mark E. McComb<sup>1</sup>; <sup>1</sup>*Boston University School of Medicine, Boston, MA*; <sup>2</sup>*Children's Hospital Oakland Research Institute, Oakland, CA*
- MP 219 **Front-End Electron Transfer Dissociation Coupled with 21 T FT-ICR MS with Data Dependent Parameter Adjustment for Top-Down Protein Analysis;** Nathan Kaiser<sup>1</sup>; Don Smith<sup>1</sup>; Chad Weisbrod<sup>1</sup>; Greg T. Blakney<sup>1</sup>; John Quinn<sup>1</sup>; Alan Marshall<sup>1,2</sup>; Chris Hendrickson<sup>1</sup>; Donald Hunt<sup>3</sup>; <sup>1</sup>*National High Magnetic Field Laboratory, Tallahassee, FL*; <sup>2</sup>*FSU Dept of Chemistry and Biochemistry, Tallahassee, FL*; <sup>3</sup>*University of Virginia, Charlottesville, VA*
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- MP 221 **Bromophenacyl-8 Reaction to Identify Highly-Polar Carboxyl-Containing Compounds in Complex Mixtures Using HPLC-Mass Spectrometry;** Quanbo Xiong; Serge Fotso; Negar Garizi; *Dow AgroSciences, Indianapolis, IN*
- MP 222 **APGC-QToF-MS of the Organic Constituents of the Nest Entrance Tubes of the Stingless Honeybee (Apidae: Meliponini);** Jeffrey Morré; Chris Beaudry; Michael Burgett; Liping Yang; Claudia Maier; *Oregon State University, Corvallis, OR*
- MP 223 **LC-MS Based Metabolite Fingerprinting and Profiling of a Traditional Chinese Medicine Formulation from Two Vendors;** Ahmad Almalki; *Auburn, AL*
- MP 224 **High Throughput Screening of Natural Products Utilizing Pulsed Ultrafiltration or MMS with UHPLC MS/MS;** Michael Rush; Elisabether Walker; Richard B. Van Breemen; *University of Illinois, Chicago, IL*
- MP 225 **Characterizing the Secondary Metabolites of *Pinus armandii* by On-Line HPLC-SPE/MS;** Yi-Lynn Chen; Kuo-Lung Ku; *National Chiayi University, Chiayi City, Taiwan*
- MP 226 **Surface MALDI-MS Imaging for the Discovery of Natural Products from Fungus-Growing Ants;** Erin Gemperline<sup>1</sup>; Heidi Horn<sup>2</sup>; Cameron Currie<sup>2</sup>; Lingjun Li<sup>1,3</sup>; <sup>1</sup>*Department of Chemistry, UW-Madison, Madison, WI*; <sup>2</sup>*Department of Bacteriology, UW-Madison, Madison, WI*; <sup>3</sup>*School of Pharmacy, UW-Madison, Madison, WI*
- MP 227 **Development of a Rapid Electrospray Ionization Mass Spectrometry Methodology for Simultaneous Determination of the Bioactive Constituents of *Vitis vinifera* L;** Andrey P. Lopes<sup>1,2</sup>; Bianca S. Bagatela<sup>1,2</sup>; Fabio F. Perazzo<sup>1</sup>; Demian R. Ifa<sup>2</sup>; <sup>1</sup>*UNIFESP, São Paulo, São Paulo*; <sup>2</sup>*York University, Toronto, Ontario*
- MP 228 **Liquid Chromatography Mass Spectrometry Based workflows for Herbal Product Analysis;** Manoj Pillai; Akanksha Singh; *SCIEX, 121, Udyog Vihar Phase IV, Gurgaon, Haryana, India*
- MP 229 **Isolation and Characterization of Quinones from *Tectona grandis* Linn. Leaves using Innovative Hyphenation of TLC-MS Interface with LC/MS/MS System;** Shailendra Rane<sup>1</sup>; Rashi Kochhar<sup>1</sup>; Shailesh Damale<sup>1</sup>; Deepti Bhandarkar<sup>1</sup>; Shruti Raju<sup>1</sup>; Ajit Datar<sup>1</sup>; Jitendra Kelkar<sup>1</sup>; Pratap Rasam<sup>1</sup>; Akshay Charegaonkar<sup>2</sup>; Prashant Hande<sup>2</sup>; Manish Hate<sup>3</sup>; <sup>1</sup>*Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*; <sup>2</sup>*Anchrom Enterprises (I) Pvt. Ltd., Mumbai, India*; <sup>3</sup>*Ramnarain Ruia College, Mumbai, India*
- MP 230 **A Capillary Electrophoresis Mass Spectrometry Method for the Analysis of Naturally Occurring Flavonoids in Herbal Supplements;** Ryan Johnson; *Lawrence, KS*
- MP 231 **Direct Analysis of the Dry Extract from the Peels of *Citrus aurantium* L. by ESI-MS Fingerprinting and HPTLC/DESI-MS Imaging;** Bianca S. Bagatela<sup>1,2</sup>; Andrey P. Lopes<sup>1,2</sup>; Fabio F. Perazzo<sup>1</sup>; Demian R. Ifa<sup>2</sup>; <sup>1</sup>*UNIFESP, São Paulo, São Paulo*; <sup>2</sup>*York University, Toronto, ON, Canada*
- MP 232 **A Novel UHPLC Orbitrap HRMS Approach for Monitoring Sulfur Fumigation Abuse in Drying Process of Traditional Chinese Medicine;** Zhe Zhou<sup>1</sup>; Min Yang<sup>2</sup>; <sup>1</sup>*Thermo Fisher Scientific, Shanghai, China*; <sup>2</sup>*Shanghai Institute of Materia Medica, Shanghai, China*
- MP 233 **Facile Structure Elucidation of Natural Products by Mass Spectrometry;** Andrew Johnson<sup>1</sup>; Ashley Sidebottom<sup>1</sup>; Erin Carlson<sup>1,2</sup>; <sup>1</sup>*Indiana University, Bloomington, IN*; <sup>2</sup>*University of Minnesota, Minneapolis, MN*
- MP 234 **High Resolution Mass Spectrometry with Automated Data Analysis to Support Late Stage Functionalization;** Yong Liu<sup>1</sup>; Fabien Fontaine<sup>2</sup>; Huifang Yao<sup>1</sup>; Ismael Zamora<sup>2</sup>; Roy Helmy<sup>1</sup>; Shane Krska<sup>1</sup>; Kevin Bateman<sup>3</sup>; <sup>1</sup>*Merck & Co., Inc., Rahway, NJ*; <sup>2</sup>*Molecular Discovery, Barcelona, Spain*; <sup>3</sup>*Merck & Co., West Point, PA*
- MP 235 **Characterization of Pyrrolizidine Alkaloids and N-oxides from Various Parts of Many Botanicals and Dietary Supplements using UHPLC-QToF-MS;** Bharathi Avula<sup>1</sup>; Satyanarayanaraju Sagi<sup>1</sup>; Yan-Hong Wang<sup>1</sup>; Jerry Zweigenbaum<sup>2</sup>; Mei Wang<sup>1</sup>; Ikhlas A. Khan<sup>1</sup>; <sup>1</sup>*NCNPR, School of Pharmacy, Univ. of MS, University, MS*; <sup>2</sup>*Agilent Technologies, Wilmington, DE*
- MP 236 **High Throughput Determination of Eight Ginsenosides from Rat Serum and Radix Ginseng Extract by UHPLC Tandem Triple Quadrupole Mass Spectrometry;** Tao Bo; Zhongxiang Zhang; *Agilent Technologies, Beijing, China*
- MP 237 **High Throughput Analysis of Anti-Fungal Paraben in Personal-Care Products at 9 Seconds per Sample using LDTD-MS/MS;** Pascal Belisle<sup>1</sup>; Serge Auger<sup>1</sup>; Gregory Blachon<sup>3</sup>; Alex Birsan<sup>1</sup>; Jean Lacoursiere<sup>1</sup>; Annie-Claude Bolduc<sup>2</sup>; Pierre Picard<sup>1</sup>; <sup>1</sup>*Phytronix Technologies Inc., Quebec, Canada*; <sup>2</sup>*Université Laval, Québec, QC*; <sup>3</sup>*Phytronix Technologies, Québec, QC*
- MP 238 **Determining Elemental Composition of Phytochemicals in Camelina Seed Meal by High Mass Accuracy and Spectral Accuracy;** Mark Berhow<sup>1</sup>; Michael Bowman<sup>1</sup>; Ming Gu<sup>2</sup>; <sup>1</sup>*USDA, ARS, NCAUR, Peoria, IL*; <sup>2</sup>*Cerno Bioscience, Yardley, PA*
- MP 239 **Utilization of a Novel Geometry Travelling Wave IMS/Q-ToF Mass Spectrometer for Natural Products Profiling;** Anthony T. Iavarone<sup>1</sup>; Ulla N. Andersen<sup>1</sup>; Darren Hewitt<sup>2</sup>; Andrew Baker<sup>3</sup>; <sup>1</sup>*UC Berkeley, Berkeley, CA*; <sup>2</sup>*Waters, Wilmslow, UK*; <sup>3</sup>*Waters, Inc., Pleasanton, CA*
- MP 240 **Mobile Phase Investigation of Positive and Negative Ion ESI Spectra of Plant Polyacetylenes during LC/MS;** David Hasman<sup>1,2</sup>; Richard W. Smith<sup>3</sup>; <sup>1</sup>*British Columbia Institute of Technology, Burnaby, British Columbia*; <sup>2</sup>*Procyon Research Inc., Vancouver, Canada*; <sup>3</sup>*Univ of Waterloo, Waterloo, ON*
- MP 241 **Application of Chemical Fingerprint Approach to Identify Gastrodiae Rhizoma in Chinese Medicine Preparations by UPLC-QTOF-MS;** Pin-Hsiu Chen; Jhe-Wei Yu; Pei-Yi Chen; Fen-Ling Lu; Chia-Fen Tsai; Hwei-Fang Cheng; *Taiwan Food and Drug Administration, Taipei, Taiwan (R.O.C)*
- MP 242 **Profiling Fungal Cultures *in situ* via the Droplet-LMJ-SSP Coupled with UPLC-PDA-HRMS-MS/MS;** Vincent Sica<sup>1</sup>; Huzefa Raja<sup>1</sup>; Cedric Pearce<sup>2</sup>; Vilmos Kertes<sup>2</sup>; Gary J. Van Berkel<sup>3</sup>; Nicholas Oberlies<sup>1</sup>; <sup>1</sup>*University of North Carolina Greensboro, Greensboro, NC*; <sup>2</sup>*Mycosynthetix, Hillsborough, NC*; <sup>3</sup>*Oak Ridge National Laboratory, Oak Ridge, TN*
- MP 243 **Nickel (II)-assisted Tadalafil Enantiomers Analysis by Electrospray Ionization Mass Spectrometry;** Lu Wang; Cuihong Sun; Su Zeng; *Zhejiang University, Hangzhou, China*
- MP 244 **Screening and Identification of Undeclared Synthetic Compounds as Adulterants using UPLC-Qtof-MS Coupled to a Novel Informatics Platform;** Dhavalkumar Narendrabhai Patel<sup>1</sup>; Lirui Qiao<sup>2</sup>; Jimmy Yuk<sup>3</sup>; Giorgis Isaac<sup>3</sup>; Kate Yu<sup>3</sup>; <sup>1</sup>*Waters Pacific Private Ltd, Singapore, Singapore*; <sup>2</sup>*Waters Corporation, Shanghai, China*; <sup>3</sup>*Waters Corporation, Milford, MA*
- MP 245 **A Comprehensive Platform for the Identification and Mode of Action Characterization of Bioactive Natural Products from Complex Libraries;** Roger G. Linington<sup>1</sup>; Kenji L. Kurita<sup>1</sup>; Giorgis Isaac<sup>2</sup>; Mark Wrona<sup>2</sup>; Kate Yu<sup>2</sup>; <sup>1</sup>*University of California Santa Cruz, Santa Cruz, CA*; <sup>2</sup>*Waters Corporation, Milford, MA*
- MP 246 **REDichips for Applied Quantitation of Alkaloids;** Haddon Goodman<sup>1</sup>; Gregory Boyce<sup>1</sup>; Daniel Panaccione<sup>2</sup>; <sup>1</sup>*Protea Biosciences, Morgantown, WV*; <sup>2</sup>*West Virginia University, Morgantown, WV*

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- MP 247 **Method Development and Validation for the Quantitation of HMF and HMFA in Human Plasma Using LC-MS/MS;** Meng Fang<sup>1</sup>; Yifan Shi<sup>1</sup>; Yinghe Li<sup>1</sup>; Michael Zhang<sup>1</sup>; Bradley Gillespie<sup>2</sup>; Warren Stern<sup>3</sup>; Amy Wang<sup>4</sup>; Nora Yang<sup>4</sup>; Xin Xu<sup>4</sup>; <sup>1</sup>Alliance Pharma Inc, Malvern, PA; <sup>2</sup>Leidos Biomedical Research Inc., Frederick, MD; <sup>3</sup>AesRx, LLC, Newton, MA; <sup>4</sup>TRND/NCATS, National Institutes of Health, Rockville, MD
- MP 248 **A Case Study for Oxcarbazepine Variation in Sample Extracts Due To Adsorption in 96-well Plates by LC-MS.**; Richard Lavallée; Georges Koudssi; Milton Furtado; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*
- MP 249 **Development and Validation of a High Throughput LC-MS/MS Method for Determination of Clobazam and N-Desmethyclobazam in Human Plasma;** Jasper X. Chu; Yuzhu Xue; Mary Hillegas; Yuan-Shek Chen; *QPS LLC, Newark, DE*
- MP 250 **Quantitative Measurement of Lovastatin and Lovastatin Acid in Human Plasma using Column Switching and Tandem Mass Spectrometry;** Jingduan Chi; Erika Helgerson; Lisa McIntosh; Fumin Li; *PPD Inc, Madison, WI*
- MP 251 **Simultaneous Quantitation of Delamanid (OPC-67683) and its Eight Metabolites in Human Plasma using UHPLC-MS/MS;** Min Meng<sup>1</sup>; Bradley Bessette<sup>1</sup>; Benjamin Smith<sup>1</sup>; Brad Johnston<sup>1</sup>; Spencer Carter<sup>1</sup>; Jerry Brisson<sup>2</sup>; Sharin E. Roth<sup>2</sup>; <sup>1</sup>Tandem Labs, Salt Lake City, UT; <sup>2</sup>Otsuka Pharmaceutical Development, Rockville, MD
- MP 252 **Increase Selectivity in Quantitative LC-MS/MS Analysis using On-line Extraction via an Analyte Interaction Exclusion Process ;** Mathieu Lahaie; Milton Furtado; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*
- MP 253 **Determination of Methamphetamine in Human Hair by Ultra High Performance Liquid Chromatography/Tandem Mass Spectrometry;** Chao Ma<sup>1</sup>; Kai Zhang<sup>2</sup>; Yumin Di<sup>2</sup>; Yueqi Li<sup>1</sup>; Guixiang Yang<sup>1</sup>; Taohong Huang<sup>1</sup>; Shin-ichi Kawano<sup>1</sup>; Yuki Hashi<sup>1</sup>; <sup>1</sup>Shimadzu Global COE, Shimadzu (China) Co., Ltd, Beijing, China; <sup>2</sup>Tianjin Public Security Bureau, Tianjin, China
- MP 254 **Identification of a Contaminant Interfering with 6-Hydroxyoxymorphone Quantification by using TOF-MS;** Eugénie-Raphaëlle Bérubé; Milton Furtado; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*
- MP 255 **Quantification of Thiazolidine-4-carboxylic Acid in Toxicant-Exposed Cells by Liquid Chromatography-Mass Spectrometry Reveals an Intrinsic Antagonistic Response to Oxidative Stress-Induced Toxicity;** Jingjing Liu; *Hong Kong, China*
- MP 256 **Quantitative Analysis of Antipsychotics in Urine by Liquid Chromatography-Triple Quadrupole Mass Spectrometry;** Flaubert Mbeunkui; Carla Lyon; R. Brent Dixon; *Physicians Choice Laboratory Services, Rock Hill, SC*
- MP 257 **Development of the Separation of Three Tyrosine Isomers in Protein Hydrolysate Samples;** Huseyin Kayadibi<sup>1,2</sup>; Tammy Bullwinkle<sup>3</sup>; Noah Reynolds<sup>3</sup>; Medha Raina<sup>3</sup>; Adil Moghal<sup>3</sup>; Eleftheria Matsa<sup>3</sup>; Andrei Rajkovic<sup>3</sup>; Farbod Fazlollahi<sup>1</sup>; Christopher Ryan<sup>1</sup>; Kym Faull<sup>1</sup>; Michael Ibba<sup>3</sup>; <sup>1</sup>UCLA, Los Angeles, CA; <sup>2</sup>Adana Military Hospital, Adana, Turkey; <sup>3</sup>Ohio State University, Columbus, OH
- MP 258 **Development and Validation of LC-MS/MS Method for Determination of N-Tetracosanoylsphinganine in Human Plasma;** Hui Jiang; Jean Schaffer; Daniel Ory; Xuntian Jiang; *Diabetic Cardiovascular Disease Center, Washington, St. Louis, MO*
- MP 259 **Matrix Effect, Sensitivity and Throughput of Microflow Liquid Chromatography vs. HPLC: A Case Study With Buprenorphine and Norbuprenorphine;** Laurence Mayrand-Provencher; Milton Furtado; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*
- MP 260 **Event Investigation of Sample Inhomogeneity in Acidified Human Plasma Samples in a First-in-Human Study;** Phillip S. Wong; Jian jiang; Christopher James; *Amgen, Thousand Oaks, CA*
- MP 261 **Quantification of Nicotine and Its Metabolite Cotinine in Human Tooth Using Triple Quad 6500 LC-MS/MS;** HongKun Wu<sup>1</sup>; Junyu Lee<sup>2</sup>; Joshua Froning<sup>2</sup>; Yong-Xi Li<sup>2</sup>; <sup>1</sup>West China Hospital of Stomatology, Chengdu, China; <sup>2</sup>Medpace Bioanalytical Laboratories, Cincinnati, OH
- MP 262 **Improved Sensitivity and Selectivity by using LC-HRMS for the Quantification of Latanoprost Acid in Dog Plasma at 5.00 pg/mL;** Richard Lavallée<sup>1</sup>; Milton Furtado<sup>1</sup>; Deepank Utkhede<sup>2,3</sup>; Fabio Garofolo<sup>1</sup>; <sup>1</sup>Algorithme Pharma Inc., Laval, Canada; <sup>2</sup>Mati Therapeutics (Canada) Inc., Burnaby, Canada; <sup>3</sup>Mati Therapeutics Inc., Austin, Texas
- MP 263 **Simultaneous Determination of 12 Volatile Organic Compounds in Human Blood by SPME-GC/MS/MS;** Zhiyun Jin<sup>1</sup>; Rocio Aranda-Rodriguez<sup>1</sup>; Ashley Cabecinha<sup>1</sup>; Jeromy Harvie<sup>1</sup>; Axelle Marchand<sup>2</sup>; Robert Tardif<sup>2</sup>; Andy Nong<sup>1</sup>; Sami Haddad<sup>2</sup>; <sup>1</sup>Health Canada, Ottawa, Canada; <sup>2</sup>Université de Montréal, Montréal, Canada
- MP 264 **Effective Carryover Reduction by Derivatization of Residual Analyte in HPLC System during LC-MS/MS Quantification;** Vinicio Vasquez; Sylvain Latour; Milton Furtado; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*
- MP 265 **Validation of a Liquid Chromatography-Tandem Mass Spectrometric Assay for Tacrolimus in Peripheral Blood Mononuclear Cells;** Min Chang Kim; Jun Hwa Shim; Hwa-Suk Kim; Seo Hyun Yoon; Kyung-Sang Yu; In Jin Jang; Joo Youn Cho; *Seoul National University, Seoul, South Korea*
- MP 266 **Overcoming Hematocrit Impact Using Homogenization Beads for Dried Blood Spots (DBS) by LC-MS/MS Analysis;** Nikolay Yuhnovski; Julien Nantel; Milton Furtado; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*
- MP 267 **A Rapid LC-MRM/MS Assay for Simultaneous Quantification of Choline, Betaine, Trimethylamine, Trimethylamine N-oxide and Creatinine;** Xueqing Zhao<sup>1</sup>; Steven Zeisel<sup>1</sup>; Shucha Zhang<sup>2</sup>; <sup>1</sup>Nutrition Research Institute, UNC Chapel Hill, Kannapolis, NC; <sup>2</sup>Brigham and Women's Hospital, Boston, MA
- MP 268 **A Validated Method for the Quantitation of Evogliptin in Human Plasma using Liquid Chromatography-Tandem Mass Spectrometry;** Jun Hwa Shim; Hwa-Suk Kim; Min Chang Kim; Seo Hyun Yoon; Kyung-Sang Yu; In-Jin Jang; Joo-Youn Cho; *Seoul National University College of Medicine, Seoul, South Korea*
- MP 269 **Evaluation of Bench-top Quadrupole Orbitrap Ultra High Resolution Mass Spectrometer for Rapid Quantitative Analysis of Immunosuppressant Drugs in Blood Samples;** Mindy Gao; Marta Kozak; *ThermoFisher Scientific, San Jose, CA*
- MP 270 **Simultaneous Quantification of Loxapine and its Four Metabolites in Human Plasma using LC-MS/MS;** Min Meng<sup>1</sup>; Benjamin Smith<sup>1</sup>; Laixin Wang<sup>1</sup>; Brad Johnston<sup>1</sup>; Scott Reuschel<sup>1</sup>; Charisse Green<sup>2</sup>; Steven H Gorman<sup>2</sup>; <sup>1</sup>Tandem Labs, Salt Lake City, UT; <sup>2</sup>Teva Branded Pharmaceutical Products R & D, Inc, West Chester, PA
- MP 271 **Quantitative Analysis of Cotinine in Human Plasma and Urine Utilizing a Simple Liquid/Liquid Extraction and GC-MS/MS;** Chad Christianson<sup>1</sup>; Ekong Basse<sup>2</sup>; Keith Miller<sup>1</sup>; <sup>1</sup>Alturas Analytics, Moscow, ID; <sup>2</sup>ThermoFisher Scientific, San Jose, CA
- MP 272 **Novel HILIC-LC-MS/MS Quantitative Method for the Bio-Analysis of Gemini Surfactants Designed as Nanomaterial Drug Carriers;** McDonald Donkuru; George Katselis; Anas El-Aneed; *University of Saskatchewan, Saskatoon, Canada*



- MP 273 **Method Validation of Quantitative Analysis of [<sup>14</sup>C] YH4808 in Human Plasma by Accelerator Mass Spectrometry;** Hwa Suk Kim<sup>1</sup>; Jun Hwa Shim<sup>1</sup>; Min Chang Kim<sup>1</sup>; Byung-Yong Yu<sup>2</sup>; Howard Lee<sup>1</sup>; In-Jin Jang<sup>1</sup>; Joo-Youn Cho<sup>1</sup>; <sup>1</sup>Seoul National University Hospital, Seoul, South Korea; <sup>2</sup>Korea Institute of Science and Technology, Seoul, South Korea
- MP 274 **Rapid Determination of Multiple Non-Steroidal Anti-Inflammatory Drugs (NSAIDs) in Microliter Quantities of Human Plasma using LC-MS/MS;** Chen Zhang; A. Daniel Jones; *Michigan State University, East Lansing, MI*
- MP 275 **Increase of Sensitivity and Precision at Low Concentration for LC-MS/MS Quantification of 11-Hydroxy-Δ<sup>9</sup>-tetrahydrocannabinol by Summation of the MRM Transitions;** Romain Beauvois; Vinicio Vasquez; Milton Furtado; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*
- MP 276 **Robust LCMSMS Determination of Intact Conjugated Dextrophan when Hydrolysis is Inefficient;** Genevieve Emond; Philippe Bélanger; Luc Bouchard; Louis-Charles Boisvert; Marie-Josée Marcoux; Nancy Lampron; Nadine Boudreau; Ann Lévesque; *InVentiv Health Clinical, Québec, Canada*
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- MP 277 **Automated *in vitro* ADME Screening Analysis in a Small Footprint, using TQ-S Micro Triple Quadrupole Mass Spectrometer;** Yun Alelyunas; Kelly Doering; Stephen McDonald; Mark Wrona; *Waters Corporation, Milford, MA*
- MP 278 **Software-Assisted Structural Characterization of Disulphide-Rich Macromolecular Peptides in Drug Discovery Research;** Asoka Ranasinghe; Eugene F. Ciccimaro; Serhiy Hnatyshyn; Celia D'Arienzo; Timothy Olah; *Bristol-Myers Squibb Company, Princeton, NJ*
- MP 279 **Comparison of Blood Microsampling Techniques for Discovery PK Studies in Rats: Capillary Microsampling (CMS) and a Dried Matrix Microsampling Device;** Walter Korfmacher<sup>1</sup>; Yongyi Luo<sup>2</sup>; Stacy Ho<sup>1</sup>; Jie Wang<sup>2</sup>; Gregory Snow<sup>3</sup>; Thomas O'Shea<sup>1</sup>; <sup>1</sup>Genzyme, Waltham, MA; <sup>2</sup>Sanofi, Waltham, MA; <sup>3</sup>Agilux Labs, Worcester, MA
- MP 280 **Expression of Drug-Adme-Associated Proteins in Human Small Intestine, Liver, and Kidney Microsomes: Swath-MS-Based Absolute Protein Quantification;** Shingo Ito<sup>1,3</sup>; Kenji Nakamura<sup>2</sup>; Mio Hirayama<sup>1,3</sup>; Sumio Ohtsuki<sup>1,3</sup>; <sup>1</sup>Fac. of Life Sci., Kumamoto Univ., Kumamoto, Japan; <sup>2</sup>Grad. Sch. of Pharma. Sci., Kumamoto Univ., Kumamoto, Japan; <sup>3</sup>CREST, JST, Kawaguchi, Japan
- MP 281 **A Mass Spectrometry Based Assay to Identify New Lead Compounds against Drug Resistant Bacterial Infections;** Daniel Todd<sup>1</sup>; David Zich<sup>1</sup>; Martha Leyte-Lugo<sup>1</sup>; Alexander Horswill<sup>2</sup>; Nadja Cech<sup>1</sup>; <sup>1</sup>Univ. of N. Carolina Greensboro, Greensboro, NC; <sup>2</sup>University of Iowa, Iowa City, IA
- MP 282 **Novel Approach for Pharmacokinetics and Protein Binding Analysis of Teneligliptin using LC-ESI-QTOF Accurate Mass Spectrometer and Ultra-filtration: *in-vitro*, *in-vivo* Correlation;** Shanti Kumar Saladi<sup>1</sup>; Prasanth B<sup>1</sup>; Veerbhadra Swamy C<sup>1</sup>; Srinivas R<sup>2</sup>; Satheesh Kumar N<sup>1</sup>; <sup>1</sup>NIPER-Hyderabad, Hyderabad, India; <sup>2</sup>National Center for Mass Spectrometry, IICT, Hyderabad, India
- MP 283 **Assessing Hemolysis Failures for LC-MS/MS Assays Using LC-HRAM on a Q-Exactive Mass Spectrometer;** Laixin Wang<sup>1</sup>; Alicia Pietrasiewicz<sup>1</sup>; Chad Moore<sup>1</sup>; Carrie Pederson<sup>1</sup>; Scott Reuschel<sup>1</sup>; Min Meng<sup>1</sup>; Hongxia Wang<sup>2</sup>; David Horn<sup>2</sup>; Jonathan Josephs<sup>2</sup>; <sup>1</sup>Tandem Labs, Salt Lake City, UT; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- MP 284 **Quantitation of Thioether-Prodrug NS1040 and Its Metabolites in Rat Plasma Using Ultra-Performance Liquid Chromatography-Tandem Mass Spectrometry;** Emma Hughes<sup>1</sup>; Daniel Appella<sup>2</sup>; Matthew Hassink<sup>2</sup>; Nathaniel Shank<sup>2</sup>; Kara George-Rosenker<sup>2</sup>; Xin Xu<sup>1</sup>; Amy Wang<sup>1</sup>; <sup>1</sup>NCATS NIH, Rockville, MD; <sup>2</sup>NIDDK NIH, Bethesda, MD
- MP 285 **Differential Mobility Spectrometry as a Measure of Physicochemical Properties Related to *in vitro* Absorption (permeability, solubility and lipophilicity);** Jefry Shields<sup>1</sup>; Chang Liu<sup>2</sup>; John Janiszewski<sup>1</sup>; Hui Zhang<sup>1</sup>; J. Larry Campbell<sup>2</sup>; J.C. Yves Leblanc<sup>2</sup>; <sup>1</sup>Pfizer Inc., Groton, CT; <sup>2</sup>AB SCIEX, Concord, ON
- MP 286 **An Ion-Pairing Strategy to Overcome PEG-400 Caused Matrix Effect in Routine Drug Discovery Blood Sample Analysis;** Linlin Dong; Michael Johnson; Mark Qian; Shaoxia Yu; *Takeda Pharmaceuticals International Co., Cambridge, MA*
- MP 287 **Evaluation of Supercritical Fluid Chromatography/Mass Spectrometry for Use in PK/PD Studies;** Fangbiao Li<sup>1</sup>; Bernard Choi<sup>1</sup>; Cynthia M. Chavez-Eng<sup>1</sup>; Christopher Kochansky<sup>1</sup>; Eric Streakfuss<sup>1</sup>; Joan Ellis<sup>1</sup>; Bang-lin Wan<sup>1</sup>; Emily Adarayan<sup>1</sup>; Brad Coopersmith<sup>2</sup>; Richard Depinto<sup>2</sup>; Isabelle Vutrieu<sup>2</sup>; Eva Gallea<sup>2</sup>; Lucinda Cohen<sup>1</sup>; Rena Zhang<sup>1</sup>; Kevin Bateman<sup>1</sup>; <sup>1</sup>Merck Research Laboratories, West Point, PA; <sup>2</sup>Waters, Richboro, PA
- MP 288 **Radio-Labeled Compound Detection Using Fine Isotopic Structures From Very High Resolution Mass Spectrometry;** Xiaojie C. Ding<sup>1</sup>; Tim Stratton<sup>2</sup>; Ji Ma<sup>3</sup>; <sup>1</sup>Thermo Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA; <sup>3</sup>Amgen Inc., South San Francisco, CA
- MP 289 **Segmentation of the Tumour Microenvironment using Multimodal Molecular Imaging to Refine PK/PD Modelling;** Jo Cappell<sup>1</sup>; Richard Goodwin<sup>2</sup>; Peter Webborn<sup>2</sup>; Ron M.A. Heeren<sup>1</sup>; <sup>1</sup>University of Maastricht, Maastricht, Netherlands; <sup>2</sup>AstraZeneca, Macclesfield, UK
- MP 290 **A Sample Preparation and Detection Strategy for Quantifying Proteolytically Unstable Therapeutic Peptides for Early-ADME Tissue Distribution Studies;** Yasmin Boukhedimi<sup>1</sup>; Aristidis Gritsas<sup>1</sup>; Garnet McRae<sup>2</sup>; Roger Leger<sup>1</sup>; Paul Drogaris<sup>1</sup>; <sup>1</sup>Thrasos therapeutics, Montreal, Canada; <sup>2</sup>G McRae Consulting, Ottawa, Canada
- MP 291 **A Sensitive Liquid Chromatography-Tandem Mass Spectrometric Method for Determination of Octreotide in Human Plasma;** Yuling Song; Jinting Yao; Hongyuan Hao; Taohong Huang; Shin-ichi Kawano; Yuki Hashi; *Shimadzu (China) Co., LTD, Shanghai, China*
- MP 292 **Antibody-Free Mass Spectrometry Workflow For Protein Expression Analysis of Intestinal Efflux Transporters in Knock Out Cell Lines;** Yongsheng Xiao; James J Walters; Maureen Bourner; David C. Thompson; Kevin Ray; *Sigma-Aldrich, St. Louis, MO*
- MP 293 **Evaluation of High Resolution Mass Spectrometry for Bioanalytical Quantitation and Simultaneous Metabolite Identification;** Matthew Zimmerman; Firat Kaya; Veronique Dartois; Brendan Prideaux; *Rutgers University, Newark, NJ*
- MP 294 **Comparison of a 4-N-hydroxycytidine Ribonucleoside Phosphoramidate Prodrug with Sofosbuvir: Interspecies Hepatocytes and Human Cardiomyocytes Metabolic Profiles;** Sijia Tao<sup>1</sup>; Franck Amblard<sup>1</sup>; Yong Jiang<sup>1</sup>; Sheida Amiralaee<sup>1</sup>; Hao Li<sup>1</sup>; Steven Coats<sup>2</sup>; Raymond Schinazi<sup>1</sup>; <sup>1</sup>Emory University School of Medicine, Atlanta, GA; <sup>2</sup>CoCrystal Pharma, Inc., Tucker, GA
- MP 295 **MS Transporter Assay for d9-ergothioneine on Carnitine/Organic Cation Transporter (OCTN1/SLC22A4);** Chien-Ming Li; Xuexiang Zhang; Wenjie Jiang; Yong Huang; *Optivia Biotechnology, Menlo Park, CA*
- MP 296 **A UHPLC-MS/MS Method for the Direct Analysis of Thymoquinone in Mouse Plasma and its Application to Pharmacokinetics;** Jinghua Zhu; Qishan Lin; *University at Albany, Rensselaer, NY*



## MONDAY POSTERS

- MP 297 **Robust and Sensitive Quantitation of Midazolam and Hydroxylmidazolam in Plasma using High Capacity UHPLC and a New Triple Quadrupole Instrument;** Craig Love<sup>1</sup>; Laura Pollum<sup>1</sup>; Smriti Kherra<sup>1</sup>; Lester Taylor<sup>1</sup>; Anabel Fandino<sup>1</sup>; Martin Greiner<sup>2</sup>; Na Pi Parra<sup>1</sup>; <sup>1</sup>Agilent Technologies, Inc., Santa Clara, CA; <sup>2</sup>Agilent Technologies, Waldbronn, Germany
- MP 298 **Evaluation of a High Resolution Accurate Mass Instrument for Discovery Microsomal Clearance and Metabolite ID Analysis;** Mustafa Varoglu<sup>1</sup>; Lieu Nguyen<sup>1</sup>; Xiaowei He<sup>1</sup>; Keith Goodman<sup>2</sup>; <sup>1</sup>Cubist Pharmaceuticals, Lexington, MA; <sup>2</sup>AB Sciex, Framingham, MA
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- MP 299 **Quantitative Measurement of Vitamin D Metabolic Distributions in Human Serum after Chemical Derivatization;** Miriam Müller; Dietrich Volmer; Saarland University, Saarbrücken, Germany
- MP 300 **Development of a Multi-Method Approach for Determining Biomarkers of Sarin Exposure using a Single Blood Sample;** Ronald Evans<sup>1</sup>; Richard Lawrence<sup>1</sup>; Michael Busch<sup>2</sup>; Ashley Fancher<sup>2</sup>; <sup>1</sup>U.S. Army ECBC, Aberdeen Proving Ground, MD; <sup>2</sup>Excet Corporation, Aberdeen Proving Ground, MD
- MP 301 **Determining the Binding Ratio of Protein-Ketamine Conjugates with Nanodiamond Mass Spectrometry and Immunizing Mice with the Conjugates;** Hsi-An Chen<sup>1</sup>; Tsong-Yung Chou<sup>2</sup>; Shun-Hsing Tuan<sup>2</sup>; Wen-Ping Peng<sup>1</sup>; <sup>1</sup>National Dong Hwa University, Shoufeng, Hualien, Taiwan; <sup>2</sup>Tzu Chi University, Hualien, Taiwan
- MP 302 **A Rapid Multi-Analyte Screening of Amino Acids and Acylcarnitines in Newborns, using Dried Blood Spots [DOCUMENT NO: IVD-MKT-012057-A];** Prem K. Gupta<sup>1</sup>; Sanjeev Pandey<sup>1</sup>; Praveen K. Sharma<sup>2</sup>; Manoj Pillai<sup>2</sup>; <sup>1</sup>Innovative Life Discovery, IMT, Manesar, Haryana, India; <sup>2</sup>Sciex, 121 Udyog Vihar, Phase IV, Gurgaon, Haryana, India
- MP 303 **Quantification of Micafungin in Human Plasma by Liquid Chromatography-Tandem Mass Spectrometry;** Sebastiano Barco; , Genoa, Italy
- MP 304 **Clinical Diagnostics of Neuronal Ceroid Lipofuscinoses on Dry Blood Spots: Development of New Cathepsin Substrates for MRM-MS Determination;** Laura Ion<sup>1</sup>; Brindusa-Alina Petre<sup>2</sup>; Thomas Braulke<sup>3</sup>; Angela Schulz<sup>3</sup>; Michael Przybylski<sup>1</sup>; <sup>1</sup>Steinbeis Centre Biopolymer Analysis and Biomedica, Ruesselsheim, Germany; <sup>2</sup>A.I. Cuza University, Iasi, Romania; <sup>3</sup>University Hospital Eppendorf, Hamburg, Germany
- MP 305 **Detection of Aldosterone in Serum by a Liquid Chromatography and Tandem Mass Spectrometry on the Shimadzu LCMS-8050 System;** Robin Karras; Danni Li; University of Minnesota, Minneapolis, MN
- MP 306 **Diagnostic Protein Quantitation of 26 Actionable Targets in Patient Biopsies using Clinical Mass Spectrometry;** Wei-Li Liao; Fabiola Cecchi; Adele Blackler; Sheeno Thyparambil; Eunkyung An; Zhichang Yang; Kathleen Bengali; Alexi Drilea; Joseph Reilly; Marlene Darfler; David Krizman; Jon Burrows; Todd Hembrough; *OncoPlex Diagnostics, Rockville, MD*
- MP 307 **Development of an SPLC/MS/MS Method for Paclitaxel and Other Compounds in Whole Blood;** Kerry Hassell<sup>1</sup>; Scott Citrowske<sup>2</sup>; Keith Waddell<sup>1</sup>; <sup>1</sup>ThermoFisher Scientific, Somerset, NJ; <sup>2</sup>Boston Scientific - MTAC, Maple Grove, MN
- MP 308 **Evaluation and Comparison of Nonderivatization and Derivatization Tandem Mass Spectrometry Methods for Multianalyte Analysis in Dried Blood Spot;** Xiaolei Xie; Marta Kozak; Thermo Fisher Scientific, San Jose, CA
- MP 309 **Quantitative 'Immuno-MS/MS' of Clinically Relevant Heterogeneous Post Translational Protein Modifications: Oxidized and Truncated Parathyroid Hormone;** Li Cui<sup>1</sup>; John Wall<sup>2</sup>; Angela Podgorski<sup>2</sup>; Fabrizio Bonelli<sup>2</sup>; Marie Philipneri<sup>3</sup>; Amy Kreig<sup>3</sup>; Mustafaa Mahmood<sup>3</sup>; Kevin Martin<sup>3</sup>; Gavin Reid<sup>1,4</sup>; <sup>1</sup>Michigan State University, East Lansing, MI; <sup>2</sup>DiaSorin Inc., Stillwater, MN; <sup>3</sup>Saint Louis University, Saint Louis, MO; <sup>4</sup>University of Melbourne, Parkville, Australia
- MP 310 **Rapid and Accurate LC-MS/MS Method for the Analysis of Nicotine, Nicotine Metabolites, and Minor Tobacco Alkaloid in Urine;** Rob Freeman; Shun-Hsin Liang; Frances Carroll; Sharon Lupo; Ty Kahler; Paul Connolly; Rick Lake; Carrie Sprout; *Restek, Bellefonte, PA*
- MP 311 **Applications of Parylene-Matrix Chips on MALDI-TOF MS for Highly Sensitive Bacterial Antibiotic Susceptibility Test and new-Born Screening Test;** Jo-Il Kim; Jong-Min Park; Joo-Yoon Noh; Jae-Chul Pyun; *Yonsei University, Seoul, South Korea*
- MP 312 **Selexlon Ion Mobility Enhances Assay Performance for the Determination of F<sub>2</sub> Isoprostane in Urine by LC-MS/MS;** Joseph Greenwood<sup>1</sup>; Jim Bruton; Jennie Ward; Daniel Hoefner; Joseph McConnell; *Health Diagnostic Laboratory, Richmond, VA*
- MP 313 **Optimization of Automated Online SPE-LC-MS/MS Used in Pain Management Drug Monitoring;** Mark J. Hayward<sup>1</sup>; Rick Youngblood<sup>1</sup>; Kim Gamble<sup>1</sup>; Martin Johnson<sup>2</sup>; Matthew Hardison<sup>2</sup>; <sup>1</sup>ITSP Solutions, Hartwell, GA; <sup>2</sup>Assurance Scientific Laboratories, Bessemer, AL
- MP 314 **Next Generation Sample Preparation for MS Analysis Of Targeted Plasma Metabolites;** Fred Regnier<sup>1,2,3</sup>; Timothy Schlabach<sup>1,2</sup>; Jinhee Kim<sup>1,2</sup>; Tim Woenker<sup>1,2</sup>; Jiri Adamec<sup>4</sup>; <sup>1</sup>Novilytic, West Lafayette, IN; <sup>2</sup>Novilytic, West Lafayette, IN; <sup>3</sup>Purdue University, Carmel, IN; <sup>4</sup>University of Nebraska, Lincoln, NE
- MP 315 **Multi-site Comparison of a High-Throughput Immuno-MALDI Plasma Renin Activity Assay with Methods Currently Used in Clinical Laboratories;** Michael Chen<sup>1</sup>; Robert Popp<sup>2</sup>; Andrew Chambers<sup>2</sup>; Shaun Eintracht<sup>1</sup>; Elizabeth McNamara<sup>1</sup>; Christoph Borchers<sup>2,3</sup>; <sup>1</sup>Dept. of Diagnostic Medicine, Jewish Gen.Hospital, Montreal, Quebec, Canada; <sup>2</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada; <sup>3</sup>Dept. of Biochem. & Microbiol., Univ. of Victoria, Victoria, BC, Canada
- MP 316 **A Direct LC/MS/MS Method for Quantitative Determination of 25-Hydroxyvitamin D2 and D3 in Human Plasma;** Zhi Wei Edwin Ting<sup>1</sup>; Jun Xiang Lee<sup>2</sup>; Jie Xing<sup>1</sup>; Zhaoqi Zhan<sup>1</sup>; <sup>1</sup>Customer Support Centre, Shimadzu (Asia Pacific) Pte Ltd, Singapore; <sup>2</sup>School of Physical & Mathematical Science, Nanyang Technological University, Singapore
- MP 317 **A Rapid and Sensitive LC-MS/MS Method for the Analysis of Free Thyroid Hormones;** Frances Carroll; Shun-Hsin Liang; Sharon Lupo; Ty Kahler; Paul Connolly; Rick Lake; Rob Freeman; Carrie Sprout; *Restek, Bellefonte, PA*
- MP 318 **Coupling of *in-vivo* Ultrasonic Neuronavigational System and Rapid Evaporative Ionization Mass Spectrometry for the Identification of Brain Tumors during Neurosurgery;** Babar Vaqas<sup>1</sup>; Julia Balog<sup>1,2</sup>; Federico Roncaroli<sup>1</sup>; Steven Pringle<sup>2</sup>; Kevin O'Neill<sup>1</sup>; Zoltan Takats<sup>1</sup>; <sup>1</sup>Imperial College London, London, UK; <sup>2</sup>Waters Corporation, Wilmslow, UK
- MP 319 **Clinical Enzymology by Paper Spray Mass Spectrometry;** Xin Yan; Xin Li; Chengsen Zhang; Cassandra Moore; Yang Xu; R. Graham Cooks; *Purdue University, West Lafayette, IN*



- MP 320 **Mass Spectrometric Profiling of Intact Proteins Desorbed from Dried Serum Spots. A Novel Approach for Clinical Diagnostics of Pregnancy Complications;** Manja Wölter<sup>1</sup>; Manuela Ruß<sup>1</sup>; Werner Rath<sup>2</sup>; Ulrich Pecks<sup>2</sup>; Michael O. Glocker<sup>1</sup>; <sup>1</sup>Proteome Center Rostock, Rostock, Germany; <sup>2</sup>Department of Obstetrics and Gynecology, Aachen, Germany
- MP 321 **Isotope-Dilution Liquid Chromatography-Tandem Mass Spectrometry Candidate Reference Measurement Procedure for 24R,25-Dihydroxyvitamin D3 in Human Serum;** Susan Tai; Michael Nelson; NIST, Gaithersburg, MD
- MP 322 **Validation of An Automated SISCAPA-MALDI-TOF-MS Workflow for Quantification of Serum Apolipoproteins A-I and B-100 in Clinical Sera;** Irene Van Den Broek<sup>1</sup>; Jan Nouta<sup>1</sup>; Morteza Razavi<sup>2</sup>; Richard Yip<sup>2</sup>; Marco Bladergroen<sup>1</sup>; Fred Romijn<sup>1</sup>; Nico Smit<sup>1</sup>; Oliver Drews<sup>3</sup>; Rainer Paape<sup>3</sup>; Detlev Suckau<sup>3</sup>; Andre Deelder<sup>1</sup>; Yuri van der Burg<sup>1</sup>; Terry Pearson<sup>2</sup>; Leigh Anderson<sup>2</sup>; Christa Cobbaert<sup>1</sup>; <sup>1</sup>LUMC, Leiden, The Netherlands; <sup>2</sup>SISCAPA Assay Technologies, Washington, DC; <sup>3</sup>Bruker Daltonics GmbH, Bremen, Germany
- MP 323 **Improved Method for the Analysis of Drugs in Oral Fluids and Urine using the Thomson eXtreme Filter Vials® by LC-MS/MS;** Lisa Wanders; Sam Ellis; Thomson Instrument Company, Oceanside, CA
- MP 324 **Influence of Isobaric Interferences on the Accuracy of Results from LC-MS/MS Analysis of Vitamin D in Human Serum;** Dietrich Volmer; Yulin Qi; Timon Geib; Pascal Schorr; Meier Florian; Saarland University, Saarbrücken, Germany
- MP 325 **Polyvinyl Fluoride Bags for Exhaled Breath by Extractive Electrospray Ionization Mass Spectrometry;** Jiuyan Zhao<sup>1</sup>; Lanlan Zhu<sup>1</sup>; Eric Handberg<sup>2</sup>; Zhiqiang Zhu<sup>2</sup>; Xiaowei Fang<sup>2</sup>; Huanwen Chen<sup>2</sup>; Wei Zhang<sup>1</sup>; <sup>1</sup>Jiangxi Key Department of Respiratory Medicine, Nanchang, China; <sup>2</sup>East China Institute of Tech., Nanchang, China
- MP 326 **Design of Optimization: How to Improve Performance of High-Volume Clinical LC/MS/MS Assays;** Andrew Lickteig; Matthew Salske; Brian Rappold; Essential Testing, LLC, Collinsville, IL
- MP 327 **Intraoperative Tissue Identification using Rapid Evaporative Ionization: Principles of Real-time MS-guided Surgery;** Julia Balog<sup>1,2</sup>; Edward R St. John<sup>2</sup>; Babar Vaqas<sup>2</sup>; James L Alexander<sup>2</sup>; David Phelps<sup>2</sup>; Mike Morris<sup>1</sup>; Steven Pringle<sup>1</sup>; Zoltan Takats<sup>2</sup>; <sup>1</sup>Waters Corporation, Wilmslow, UK; <sup>2</sup>Imperial College London, London, UK
- MP 328 **Separation and Low Level Determination Of Thyroid Hormones From Human Serum By UHPLC-MS/MS Using A Novel C18-Based Stationary Phase;** Alan P. Mckeown<sup>1</sup>; Geoffrey Faden<sup>2</sup>; <sup>1</sup>Advanced Chromatography Technologies Ltd, Aberdeen, UK; <sup>2</sup>MACMOD Analytical Inc., Chadds Ford, PA
- MP 329 **Total Cholesterol and HDL Cross Validation between High Throughput LDTD-MS/MS Method and Reference Enzymatic Technique Used in Clinical Laboratory;** Jean Lacoursière<sup>1</sup>; Annie-Claude Bolduc<sup>2</sup>; Gregory Blachon<sup>3</sup>; Serge Auger<sup>1</sup>; Alex Birsan<sup>1</sup>; Pierre Picard<sup>1</sup>; <sup>1</sup>Phytronix Technologies Inc., Quebec, Canada; <sup>2</sup>Université Laval, Québec, QC; <sup>3</sup>Phytronix Technologies, Québec, QC
- MP 330 **The Analysis of Fentanyl and Its Analogues in Human Urine by LC-MS/MS;** Paul Connolly; Shun-Hsin Liang; Frances Carroll; Sharon Lupo; Ty Kahler; Rick Lake; Rob Freeman; Carrie Sprout; Restek, Bellefonte, PA
- MP 331 **Direct Metabolic Phenotyping of Newborns at the Molecular Level by High Resolution Mass Spectrometry Analysis of Exhaled Breath;** Vladimir Frankevich<sup>1</sup>; Nataliia Starodubtceva<sup>1</sup>; Igor Popov<sup>1</sup>; Alexey Kononikhin<sup>1</sup>; Anna Bugrova<sup>1</sup>; Stanislav Pekov<sup>1</sup>; Eugene Nikolaev<sup>2</sup>; <sup>1</sup>Federal State Budget Institution "Research Center, Moscow, RU; <sup>2</sup>Institute for Energy Problems of Chemical Physics, Moscow, RU
- MP 332 **A Dilute and Shoot FI-MS/MS Method for Quantification of Glycocholic Acid and Bilirubin in Bile;** Ramakrishna Reddy Vogguru<sup>1</sup>; Raghavi Kakarla<sup>1</sup>; Janet R Donaldson<sup>2</sup>; Baochuan Guo<sup>1</sup>; <sup>1</sup>Cleveland State University, Cleveland, Ohio; <sup>2</sup>Mississippi State University, Starkville, MS
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- MP 333 **The Use of Variable Windows LC-SWATH-MS for Improved Detection and Quantification of Human Urine Metabolites;** Gerard Hopfgartner<sup>1</sup>; Aivett Bilbao<sup>1,2</sup>; Tobias Bruderer<sup>1</sup>; Sandra Jahn<sup>1</sup>; Emmanuel Varesio<sup>1</sup>; <sup>1</sup>University of Geneva, Geneva, Switzerland; <sup>2</sup>Swiss Institute of Bioinformatics, Geneva, Switzerland
- MP 334 **Metabolite Profiling can be Used for the Classification and Understanding of the Taxonomic Relationships within Chinese Native Citrus Species;** Li Jing<sup>1</sup>; Zhentian Lei<sup>1</sup>; Guiwei Zhang<sup>2</sup>; Alan Cesar Pilon<sup>3</sup>; David V. Huhman<sup>1</sup>; Rangjin Xie<sup>2</sup>; Wanpeng Xi<sup>2</sup>; Zhiqin Zhou<sup>2</sup>; Lloyd W. Sumner<sup>1</sup>; <sup>1</sup>Samuel Roberts Noble Foundation, Ardmore, OK; <sup>2</sup>Southwest University, Chongqing, China; <sup>3</sup>São Paulo State University, São Paulo, Brazil
- MP 335 **Metabolomics Studies Paradigm Shift with Quantification: Integrating Untargeted Profiling, Targeted and Pseudo-Targeted Analysis on One Platform;** Zeming Wu<sup>1</sup>; Huichang Bi<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific (China), Shanghai, China; <sup>2</sup>School of Pharmaceutical, Sun Yat-Sen University, Guangzhou, China
- MP 336 **MRManalyzer: An Integrated Targeted Metabolomic Platform for High-Throughput Metabolite Profiling and Automated Data Processing;** Yuping Cai; Kai Weng; Yuan Guo; Zhenqiang Zhu; Chinese Academy of Sciences, Shanghai, China
- MP 337 **Effects of Senescence and Water-Stress on Soybean Metabolomics: A High-Resolution Mass Spectrometry Investigation;** William Friesen<sup>1</sup>; Ali Yilmaz<sup>2</sup>; Raymond Mutava<sup>3</sup>; Silvas Prince<sup>3</sup>; Babu Valliyodan<sup>3</sup>; Henry Nguyen<sup>3</sup>; Troy Wood<sup>1</sup>; <sup>1</sup>SUNY at Buffalo, Buffalo, NY; <sup>2</sup>University of Southampton, Southampton, UK; <sup>3</sup>University of Missouri, Columbia, MO
- MP 338 **Intact Metabolome Analysis of Mice Liver by Probe Electrospray Ionization-Tandem Mass Spectrometry (PESI-MS/MS);** Yumi Hayashi<sup>1,2</sup>; Kei Zaitsumi<sup>1,2</sup>; Tasuku Murata<sup>3</sup>; Hiroki Nakajima<sup>3</sup>; Tamie Nakajima<sup>4</sup>; Hitoshi Tsuchihashi<sup>1</sup>; Akira Ishii<sup>1</sup>; Tetsuya Ishikawa<sup>1</sup>; <sup>1</sup>Nagoya University Graduate School of Medicine, Nagoya, Japan; <sup>2</sup>Institute for Advanced Research, Nagoya University, Nagoya, Japan; <sup>3</sup>Shimadzu Corporation, Kyoto, Japan; <sup>4</sup>Chubu University, Kasugai, Japan
- MP 339 **Quantification of Oxidative Stress Metabolites in Human Serum by Liquid Chromatography Tandem Mass Spectrometry Reveals Beneficial Effects of Mediterranean Diet;** Maria G. Kakkoura<sup>1,2</sup>; Kleitos Sokratous<sup>1</sup>; Christiana Demetriou<sup>1</sup>; Maria A. Loizidou<sup>1</sup>; Andreas Hadjisavvas<sup>1,2</sup>; Kyriacos Kyriacou<sup>1,2</sup>; <sup>1</sup>Cyprus Institute of Neurology and Genetics, Nicosia, Cyprus; <sup>2</sup>Cyprus School of Molecular Medicine, Nicosia, Cyprus
- MP 340 **Can 2-deoxyglucose be metabolized? An Isotope-Based Metabolomic Analysis;** Susan Gelman; Ying-Jr Amanda Chen; Jacob Schaefer; Gary J. Patti; Washington University in St. Louis, St. Louis, MO
- MP 341 **Targeted Metabolic Profiling using High-Resolution Accurate Mass Database to Identify and Confirm Potential Biomarkers in Rose and Sunflower Plant Extracts;** Jeffrey D. Miller<sup>1</sup>; Cyrus Papan<sup>2</sup>; Jens Pfannstiel<sup>3</sup>; Iris Klaiber<sup>3</sup>; Baljit K. Ubhi<sup>4</sup>; Fadi Abdi<sup>1</sup>; Tobias Bruderer<sup>5</sup>; Emmanuel Varesio<sup>5</sup>; Gerard Hopfgartner<sup>5</sup>; <sup>1</sup>SCIEX, Framingham, MA; <sup>2</sup>SCIEX, Darmstadt, Germany; <sup>3</sup>Universität Hohenheim, Stuttgart, Germany; <sup>4</sup>SCIEX, Redwood City, CA; <sup>5</sup>University of Geneva, Geneva, Switzerland

- MP 342 **Comparison of Orthogonal Column Chemistries and Ionization Polarity for Increased High Resolution Metabolome (HRM) Coverage;** [Vilinh Tran](#); Douglas Walker; Karan Uppal; Shuzhao Li; Sophia Banton; Dean Jones; *Clinical Biomarker, Emory School of Medicine, Atlanta, GA*
- MP 343 **Expanding the Coverage of Metabolome Using Multiple Liquid Chromatography Modes;** [Junhua Wang](#)<sup>1</sup>; Gina Tan<sup>1</sup>; Xiaodong Liu<sup>2</sup>; Yingying Huang<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific Inc, San Jose, CA*; <sup>2</sup>*Thermo Fisher Scientific, Sunnyvale, CA*
- MP 344 **LC-MS/MS Monitoring of the Knockout of Lysine Dehydrogenase and Amino adipic Semialdehyde Dehydrogenase in *Ruegeria pomeroyi*;** Izabella A. Pena Neshich<sup>1</sup>; [Lygia Marques](#)<sup>2</sup>; Marcos Eberlin<sup>2</sup>; Paulo Arruda<sup>1,3</sup>; <sup>1</sup>*Centro de Biologia Molecular e Engenharia Genética, Campinas, Brazil*; <sup>2</sup>*Laboratório ThoMSon de Espectrometria de Massas, Campinas, Brazil*; <sup>3</sup>*Departamento de Genética e Evolução, Campinas, Brazil*
- MP 345 **Validation of a Retention Time Accurate Mass Library for Semi-Polar Metabolites using Open Source MS-DIAL Software and NIST MS PepSearch;** [Stephanie Samra](#); Ingrid Gennity; Megan Showalter; Oliver Fiehn; *UC Davis, Davis, CA*
- MP 346 **Determination of Intracellular Metabolites by Ion-Paring Liquid Chromatography-Mass Spectrometry;** [Lili Guo](#); Andrew Worth; Clementina Mesaros; Ian A. Blair; *University of Pennsylvania, Philadelphia, PA*
- MP 347 **Metabolomics Method to Comprehensively Analyze Amino Acids in Different Domains;** [Haiwei Gu](#)<sup>1,2</sup>; Jianhai Du<sup>1</sup>; Fausto Carnevale Neto<sup>1,3</sup>; Patrick Carroll<sup>4</sup>; Sally Turner<sup>1</sup>; Gabriela Chiorean<sup>1,5</sup>; Robert Eisenman<sup>4</sup>; Daniel Raftery<sup>1,4</sup>; <sup>1</sup>*University of Washington, Seattle, WA*; <sup>2</sup>*East China Institute of Technology, Nanchang, China*; <sup>3</sup>*Sao Paulo State University, Araraquara, Brazil*; <sup>4</sup>*Fred Hutchinson Cancer Research Center, Seattle, WA*; <sup>5</sup>*Indiana University Melvin and Bren Simon Cancer Ce, Indianapolis, IN*
- MP 348 **Application of Metabolic Transistor Strategy to Control Electron Transfer Chain Function in *Escherichia coli* by Manipulating Quinone Synthesis Pathway;** [Leepika Tuli](#)<sup>2</sup>; Hui Wu<sup>1</sup>; George Bennett<sup>2</sup>; Ka-Yiu San<sup>2</sup>; <sup>1</sup>*State Key Laboratory of Bioreactor Engineering, Shanghai, China*; <sup>2</sup>*Rice University, Houston, TX*
- MP 349 **A Metabolomic Comparison of Primary and Immortalized Cells of the Same Lineage;** [Jessica Lloyd Genenbacher](#); Gary J. Patti; *Washington University, Saint Louis, MO*
- MP 350 **Quantitative Profiling of Specialized Metabolites from Transgenic Lines of *Camptotheca acuminata* using Liquid Chromatography, Multiplexed CID and Time-of-Flight Mass Spectrometry;** [Sujana Pradhan](#); Radin Sadre; Maria Magallanes-Lundback; Vonny Salim; Dean DellaPenna; A. Daniel Jones; *Michigan State University, East Lansing, MI*
- MP 351 **Construction of a Metabolite MS/MS Library for Laser Desorption Ionization Mass Spectrometry from Silicon Nanopost Arrays;** [Andrew Korte](#)<sup>1</sup>; Nicholas Morris<sup>2</sup>; Trust Razunguzwa<sup>2</sup>; Akos Vertes<sup>1</sup>; <sup>1</sup>*George Washington University, Washington, DC*; <sup>2</sup>*Protea Biosciences Inc., Morgantown, WV*
- MP 352 **Understanding the Contribution of Glutamine in Fatty Acid Biosynthesis using <sup>13</sup>C-stable Labelled Metabolites in Conjunction with an Integrated High-Throughput Methodology;** [Darren Dumlao](#)<sup>1</sup>; Mary Piotrowski<sup>1</sup>; Jefry Shields<sup>1</sup>; Richard Kibbey<sup>2</sup>; John Janiszewski<sup>1</sup>; Russell Miller<sup>3</sup>; Min Wan<sup>3</sup>; <sup>1</sup>*Pfizer, Inc, Groton, CT*; <sup>2</sup>*Yale School of Medicine, New Haven, CT*; <sup>3</sup>*Pfizer, Inc, Cambridge, MA*
- MP 353 **Investigation of Imidacloprid toxicity on the central nervous system of the snail *Lymnaea stagnalis* by targeted Metabolomics;** Sara Tufi<sup>1</sup>; Marja H. Lamoree<sup>1</sup>; [Christian Ravensborg](#)<sup>2</sup>; Aiko Barsch<sup>2</sup>; Pim E.G. Leonards<sup>1</sup>; <sup>1</sup>*Institute for Environmental Studies, VU University, Amsterdam, Netherlands*; <sup>2</sup>*Bruker Daltonics, Bremen, Germany*
- MP 354 **High-Performance Chemical Isotope Labeling Liquid Chromatography Mass Spectrometry for Investigating the Effect of Drinking Red Wine on Urine Metabolome;** [Yunong Li](#); Liang Li; *UAlberta, Edmonton, Canada*
- MP 355 **<sup>13</sup>C Glucose Infusion in Human Subjects: Metabolomic analysis in the Q Exactive;** Stephen B. Harvey; *University of Minnesota, Minneapolis, MN*
- MP 356 **An Interactive Digital Pathway Map: A Resource for Interpreting Metabolomic Data;** [Nick Spittler](#)<sup>1,2</sup>; Fuad Naser<sup>1,2</sup>; Gary J Patti<sup>1</sup>; <sup>1</sup>*Washington University in St. Louis, St. Louis, MO*; <sup>2</sup>*Connex, St. Louis, MO*
- MP 357 **Uncovering Metabolic Changes in Single *Drosophila melanogaster* infected by Nematode Parasites using Capillary Electrophoresis Mass Spectrometry;** [Sam Choi](#); Rosemary Onjiko; Shruti Yadav; Ioannis Eleftherianos; Peter Nemes; *George Washington University, Washington, DC*
- MP 358 **Development of a Chromatographic Screening Approach for Metabolomic Profiling;** [Thomas Horvath](#); Michael Pontikos; David Hawke; Phil Lorenzi; John Weinstein; *University of Texas MD Anderson Cancer Center, Houston, TX*
- MP 359 **Detection and Annotation of the Small Molecule Fraction of Soil Organic Matter;** [Stefan Jenkins](#); Peter Andeer; Tami Swenson; Trent Northen; *Lawrence Berkeley National Laboratory, Berkeley, CA*
- MP 360 **Determining Nutrient Utilization Rates Without Isotopes in Early Zebrafish Development;** [Jonathan Spalding](#)<sup>1,2</sup>; Anna Chen<sup>1,2</sup>; Nathaniel Mahieu<sup>1</sup>; Stephen Johnson<sup>2</sup>; Gary Patti<sup>1,3</sup>; <sup>1</sup>*Department of Chemistry, Washington University, St. Louis, MO*; <sup>2</sup>*Department of Genetics, Washington University, St. Louis, MO*; <sup>3</sup>*Department of Medicine, Washington University, St. Louis, MO*
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- MP 361 **Coupling Liquid-Phase Microextraction with Paper Spray for Rapid Analysis of Malachite Green, Crystal Violet, and Their Metabolites Using Mass Spectrometry;** [Jiewei Deng](#)<sup>1</sup>; Yuan Yu<sup>1</sup>; Yunyun Yang<sup>2</sup>; Xiaowei Wang<sup>1</sup>; [Tiangang Luan](#)<sup>1</sup>; <sup>1</sup>*Sun Yat-Sen University, Guangzhou, China*; <sup>2</sup>*China National Analytical Center Guangzhou, Guangzhou, China*
- MP 362 **Tissue Sample Preparation Optimization for Global Lipidomics by LC-MS;** [Danielle McDougall](#); Rainey Patterson; Yu-Hsuan Tsai; Timothy J Garrett; Richard A Yost; *University of Florida, Gainesville, FL*
- MP 363 **Separating the Separation; Evaluation of  $\mu$ -solid-phase extraction for On-Column Derivatization and Direct Injection Mass Spectrometry Sample Preparation;** [Jessica Pandohee](#)<sup>1</sup>; Andrew Minett<sup>2</sup>; Oliver A.H Jones<sup>1</sup>; <sup>1</sup>*ACROSS, School of Applied Sciences, RMIT University, Melbourne, Australia*; <sup>2</sup>*EPREP Pty Ltd, Mulgrave, Australia*
- MP 364 **Desalting of Underivatized Small Metabolites on Fluorocarbon Coated Nanoporous Silicon for Solid Matrix-Free LDI-MS (SMALDI-MS);** [Ya Zhou](#)<sup>1</sup>; Peng Chen<sup>1</sup>; D. Jed Harrison<sup>1,2</sup>; <sup>1</sup>*Department of Chemistry, University of Alberta, Edmonton, Canada*; <sup>2</sup>*National Institute for Nanotechnology, Edmonton, Canada*
- MP 365 **Quantitative Targeted Metabolomics using Dried Plasma Spots Cards;** [Kristaps Klavins](#); [Guido Dallmann](#); Therese Koal; *Biocrates Life Sciences AG, Innsbruck, Austria*



- MP 366 **Variations of Human Blood Metabolome Depending on the Employed Sampling Techniques;** Kristaps Klavins; Guido Dallmann; Therese Koal; *Biocrates Life Sciences AG, Innsbruck, Austria*
- MP 367 **Influence of Sample Preparation and Extraction Steps on Metabolomics Analysis of *Elaeis guineensis* Leaves using LC-MS;** Luiz Henrique Vargas<sup>1</sup>; José Ribeiro<sup>2</sup>; Daniel Sifuentes<sup>2</sup>; Anselmo Oliveira<sup>3</sup>; Manoel Souza Junior<sup>2</sup>; Clenilson Rodrigues<sup>2</sup>; Patrícia Verardi Abdelnur<sup>2</sup>; <sup>1</sup>*University of Lavras, Lavras, Brazil*; <sup>2</sup>*Embrapa Agroenergy, Brasília, Brazil*; <sup>3</sup>*University of Goiás, Goiânia, Brazil*
- MP 368 **The Non-Target Metabolomics of Rice Profiling Analysis by ultra-High Performance Liquid Chromatography / High-Resolution Mass Spectrometry;** Yue Song<sup>1</sup>; Chaoyang Hu<sup>2</sup>; Jianxin Shi<sup>2</sup>; Sifan Li<sup>2</sup>; Dabing Zhang<sup>2</sup>; Lei Wang<sup>3</sup>; Shan-An Chan<sup>4</sup>; <sup>1</sup>*Agilent, Shanghai, China*; <sup>2</sup>*Shanghai Nature Standard R&D and Biotech Co., Ltd., Shanghai, China*; <sup>3</sup>*Agilent, Beijing, China*; <sup>4</sup>*Agilent, Taipei, Taiwan*
- MP 369 **Derivatization of Amino Acids for Solid Matrix Laser Desorption/Ionization (SMALDI) Mass Spectrometry Analysis;** Jing Ji<sup>1</sup>; D. Jed Harrison<sup>1,2</sup>; <sup>1</sup>*Department of Chemistry, University of Alberta, Edmonton, Canada*; <sup>2</sup>*National Institute of Nanotechnology, Edmonton, Canada*
- MP 370 **Automated Metabolite Profiling in Urine by GC-MS with EI, PICI and APCI Ionization;** Martin Moos<sup>1</sup>; Kamil Petrus<sup>2</sup>; Jan Fesl<sup>1</sup>; Petr Hušek<sup>1,3</sup>; Iva Opekarová<sup>1</sup>; Helena Zahradníčková<sup>1</sup>; Ladislav Náměstek<sup>2</sup>; Petr Simek<sup>1</sup>; <sup>1</sup>*Biology Centre AS CR, Ceske Budejovice, Czech Republic, Europe*; <sup>2</sup>*Pragolab s.r.o., Prague, Czech Republic*; <sup>3</sup>*Faculty Hospital Ostrava, Ostrava, Czech Republic*
- MP 371 **High Throughput Analysis of Secondary Metabolites Excreted by Actinobacillus Isolates using Robotics and LC-MS/MS;** Leslie Silva<sup>1</sup>; Trent Northen<sup>2</sup>; <sup>1</sup>*Lawrence Berkeley National Lab, Walnut Creek, CA*; <sup>2</sup>*Lawrence Berkeley National Lab, Berkeley, CA*
- MP 372 **Systematic Comparison of Recovery and Selectivity of Liquid-Based, Solid-Phase and Size-Exclusion Extraction Methods for Global LC-MS Metabolomics of Human Plasma;** Dmitri Sitnikov; Cian Monnin; Dajana Vuckovic; *Concordia University, Montreal, Canada*
- MP 373 **An Optimized Method for Extraction of Red Blood Cell Metabolites;** Mike Williams<sup>1</sup>; Ann Guggisberg<sup>2</sup>; Christopher Beecher<sup>1</sup>; Audrey Odom<sup>2</sup>; Timothy Garrett<sup>1</sup>; <sup>1</sup>*University of Florida, Gainesville, Florida*; <sup>2</sup>*Washington University School of Medicine, St. Louis, MO*
- MP 374 **Matrix Effect on Chemical Isotope Labeling and Its Implication in Metabolomic Sample Preparation for Quantitative Metabolomics;** Wei Han; Liang Li; *University of Alberta, Edmonton, Canada*
- MP 375 **Comprehensive Human Fecal Metabolome Analysis Using Chemical Isotope Labeling LC-MS;** Nan Wang<sup>1</sup>; Wei Xu<sup>1</sup>; Deying Chen<sup>1</sup>; Xiaoling Su<sup>1</sup>; Tao Huan<sup>2</sup>; Yingfeng Lu<sup>1</sup>; Liang Li<sup>2</sup>; Lanjuan Li<sup>1</sup>; <sup>1</sup>*The First Affiliated Hospital, Zhejiang University, Hangzhou, China*; <sup>2</sup>*Department of Chemistry, University of Alberta, Edmonton, AB*
- MP 376 **Development of a Robotic Platform for Automated GCMS and LCMS Sample Preparation and Large-scale Plant Metabolomics;** David V. Huhman<sup>1</sup>; Nicky Eastham<sup>2</sup>; Graham Ellison<sup>2</sup>; Robert Talintyre<sup>2</sup>; Mike Parnell<sup>2</sup>; Li Jing<sup>1</sup>; Shelagh Henson<sup>1</sup>; Andrew Whitwell<sup>2</sup>; Lloyd Sumner<sup>1</sup>; <sup>1</sup>*The Samuel Roberts Noble Foundation, Ardmore, OK*; <sup>2</sup>*Labman Automation LTD, Seamer Hill, Stokesley, Middlesbrough, UK*
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- MP 377 **Simultaneous Quantitation of Low-Molecular Weight Sugars and Carboxylates in Wine by 3-nitrophenylhydrazine Chemical Derivatization - LC-MS/MS;** Jun Han<sup>1</sup>; Karen Lin<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>*University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada*; <sup>2</sup>*Dept. of Biochem. & Microbiol., Univ. of Victoria, Victoria, BC, Canada*
- MP 378 **Detection of Urinary Corticosteroids Metabolites by Gas Chromatography-Isotope Ratio Mass Spectrometry in Doping Control Analyses;** Xavier De La Torre<sup>1</sup>; Marta Cilia<sup>1</sup>; Davide Curcio<sup>1</sup>; Cristiana Colamonic<sup>1</sup>; Francesco Molaioni<sup>1</sup>; Daniel Jardines<sup>1</sup>; Francesco Botrè<sup>1,2</sup>; <sup>1</sup>*Laboratorio Antidoping FMSI, Rome, Italy*; <sup>2</sup>*Dipartimento di Medicina Sperimentale, "Sapienza", Rome, Italy*
- MP 379 **Identification and Characterization of Changes in Free Amino Acid and Dipeptide Concentrations in Body Fluids in Early Alzheimer's Disease;** Katherine Castor; Alfred Fonteh; Michael Harrington; *HMRI, Pasadena, CA*
- MP 380 **Combining DiLeu Isobaric Labeling and Label-free Approaches for Metabolite Quantification and Biomarker Discovery of Lower Urinary Tract Symptoms (LUTS);** Ling Hao<sup>1</sup>; Tyler Greer<sup>2</sup>; Xuefei Zhong<sup>1</sup>; David Page<sup>3</sup>; Sanghee Lee<sup>4</sup>; Chad Vezina<sup>5</sup>; Will Ricke<sup>6</sup>; Paul Marker<sup>1</sup>; Dale Bjorling<sup>6</sup>; Wade Bushman<sup>4</sup>; Lingjun Li<sup>1,2</sup>; <sup>1</sup>*School of Pharmacy, University of Wisconsin-Madison, WI*; <sup>2</sup>*Department of Chemistry, UW-Madison, WI*; <sup>3</sup>*Department of Biostatistics & Medical Informatics, UW-Madison, WI*; <sup>4</sup>*Department of Urology, UW-Madison, WI*; <sup>5</sup>*School of Veterinary Medicine, UW-Madison, WI*
- MP 381 **Ensuring Quantitative Data Reproducibility Within and Across Metabolomics Projects: Evaluation and Implementation of a Standard Quality Control for Serum/Plasma Metabolomics;** Lisa St John Williams; J Will Thompson; Laura Dubois; M Arthur Moseley; *Duke University, Durham, NC*
- MP 382 **<sup>12</sup>C/<sup>13</sup>C-labeled 3-nitrophenylhydrazine for Chemical Derivatization – UPLC-MS/MS Quantitation of Aldehyde Biomarkers of Oxidative Stress in Human Plasma;** Constance Sobsey<sup>1</sup>; Jun Han<sup>1</sup>; Karen Lin<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>*University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada*; <sup>2</sup>*Dept. of Biochem. and Microbiol., Univ. of Victoria, Victoria, BC, Canada*
- MP 383 **Quantitative and Targeted MRM-based Metabolomics Applications to Characterize Toxicity and AOP in a Zebrafish Larvae Exposure Model;** Bharat Chandramouli<sup>1</sup>; Jonathan P. Benskin<sup>2</sup>; Susie SY Huang<sup>1</sup>; John R. Cosgrove<sup>1</sup>; <sup>1</sup>*Axys Analytical Services, Ltd., Sidney, CA*; <sup>2</sup>*Stockholm University, Stockholm, Sweden*
- MP 384 **Comprehensive Analysis of Primary Metabolites by using Both Ion Pairing Chromatography and Non-Ion Pairing Chromatography;** Tsuyoshi Nakanishi<sup>1</sup>; Takako Hishiki<sup>2</sup>; Makoto Suematsu<sup>2,3</sup>; <sup>1</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>2</sup>*Keio University, Tokyo, Japan*; <sup>3</sup>*JST ERATO Suematsu Gas Biology Project, Tokyo, Japan*
- MP 385 **An Approach to Overcome Ion Suppression for Small Molecule Profiling with LC-TOF MS using Post-Column Addition;** Oskar González<sup>1,4</sup>; Frans Van der Kloet<sup>1,3</sup>; Carola Damen<sup>1,5</sup>; Rob J. Vreeken<sup>1,2</sup>; Amy Harms<sup>1</sup>; Thomas Hankemeier<sup>1</sup>; <sup>1</sup>*Leiden University, Leiden, Netherlands*; <sup>2</sup>*Janssen Pharmaceutical, Beerse, BELGIUM*; <sup>3</sup>*University of Amsterdam, Amsterdam, NL*; <sup>4</sup>*University of the Basque Country, Leioa, SP*; <sup>5</sup>*Waters, Manchester, UK*
- MP 386 **Utilization of Alkyl Maleimide Tags for Quantitation Thiol Metabolite;** Xiaofeng Zhao; *Saint Louis, MO*



## MONDAY POSTERS

- MP 387 **Quantitative LC-MS/MS Analysis of Polyamines and Their Metabolic Precursors in Lung Tissue;** Karolina M. Krasinska<sup>1</sup>; Yue Xu<sup>2</sup>; Chuong Hoang<sup>2</sup>; Allis S. Chien<sup>1</sup>; <sup>1</sup>SUMS, Stanford University, Stanford, CA; <sup>2</sup>Dept. of Thoracic Surgery, School of Medicine, Stanford, CA
- MP 388 **Development of LC-MS/MS Methods for the Targeted Analysis of Urine Metabolites Associated with Respiratory Illnesses;** Mona Khamis<sup>1,2</sup>; Hanan Awad<sup>1</sup>; Kevin Allen<sup>1</sup>; Darryl Adamko<sup>1</sup>; Anas El-Aneel<sup>1</sup>; <sup>1</sup>University of Saskatchewan, Saskatoon, Canada; <sup>2</sup>Alexandria University, Alexandria, Egypt
- MP 389 **Quantitative and Qualitative Metabolomics for the Investigation of Intracellular Metabolism;** Brigitte Simons<sup>1</sup>; Baljit Ubhi<sup>2</sup>; Douglas McCloskey<sup>3</sup>; <sup>1</sup>SCIEX, Concord, Canada; <sup>2</sup>SCIEX, Redwood City, CA; <sup>3</sup>University of California San Diego, La Jolla, CA
- MP 390 **Metabolic Effect of Drought Stress during the Grain Filling Growth Stage in Wheat Measured by Isotopic Ratio Outlier Analysis (IROA);** Felice De Jong<sup>1</sup>; Chris Beecher<sup>2</sup>; <sup>1</sup>IROA Technologies LLC, Bolton, MA; <sup>2</sup>University of Florida, Gainesville, FL
- MP 391 **Reproducible and Standardized Quantitative Bile Acids Phenotyping using UHPLC-ESI-MS/MS – International Ring Trial and Applications in Other Biologically Relevant Matrices;** Hai Pham Tuan; Doreen Kirchberg; Ines Zitturi; Therese Koal; <sup>1</sup>BIOCRATES Life Sciences AG, Innsbruck, Austria
- MP 392 **Quantification of Genitourinary Cancer Metabolites using Liquid Chromatography Triple Quadrupole Mass Spectrometry;** Sumankalai Ramachandran; Xin-Qiao Zhang; Sankar Maity; Zhen Cai; Hui-Kuan Lin; Zahi Mitri; Jianjun Gao; Timothy Thompson; Christopher Logothetics; Eleni Efsthathiou; Mark Titus; <sup>1</sup>University of Texas MD Anderson Cancer Center, Houston, TX
- MP 393 **Automated LC/MS/MS Methods Development for Targeted Bioanalysis of Metabolic Intermediates;** John Janiszewski<sup>1</sup>; Mary Piotrowski<sup>1</sup>; Brendon Kapinos<sup>1</sup>; Hui Zhang<sup>1</sup>; Darren Dumlaio<sup>1</sup>; Wayne Lootsma<sup>2</sup>; Joseph Janiszewski<sup>2</sup>; Steven Ainley<sup>2</sup>; <sup>1</sup>Pfizer Inc., Groton, CT; <sup>2</sup>Sound Analytics, East Lyme, CT
- MP 394 **A Kit for Mass-Spectrometry Based Absolute Quantification of Metabolic Enzymes;** Guido Mastrobuoni<sup>1</sup>; Fabian Bindel<sup>1</sup>; Karsten Schnatbaum<sup>2</sup>; Paul Enslé<sup>2</sup>; Julia Avramova-Nehmer<sup>2</sup>; Holger Wenschuh<sup>2</sup>; Ulf Reimer<sup>2</sup>; Stefan Kempa<sup>1</sup>; <sup>1</sup>Berlin Institute for Medical Systems Biology, Berlin, Germany; <sup>2</sup>JPT Peptide Technologies GmbH, Berlin, Germany
- MP 395 **Quantitative Analysis of Intracellular Metabolites of Microorganisms using Hyphenated Hydrophilic Interaction Liquid Chromatography Tandem Mass Spectrometry;** Reza Maleki Seifar; Cor Ras; Joseph J. Heijnen; <sup>1</sup>Delft University of Technology, Dept. Biotechnology, Delft, The Netherlands
- MP 396 **Using Open Source MZmine Software for Targeted GC-MS Data Analysis in Plasma Samples;** Martha Zuluaga<sup>1</sup>; Mimi Doll<sup>2</sup>; Luis Valdiviezo<sup>2</sup>; Lana Amerie<sup>2</sup>; Nutan Kaushik<sup>3</sup>; Oliver Fiehn<sup>2</sup>; <sup>1</sup>University of Caldas, Manizales, Colombia; <sup>2</sup>NIH West Coast Metabolomics Center UC Davis, Davis, CA; <sup>3</sup>The Energy and Resource Institute (TERI), New Delhi, India
- MP 397 **Comprehensive Analysis of Primary & Secondary Metabolites in Citrus using an Automated Method Changeover UHPLC System Coupled to LC/MS/MS;** Yuka Fujito; Kiyomi Arakawa; Yoshihiro Hayakawa; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan
- MP 398 **Quantitative Metabolomics: Way to Understand the Planarian Regeneration;** Kannan Rangiah<sup>1</sup>; Nivedita Natarajan<sup>1</sup>; Padma Ramakrishnan<sup>1</sup>; Vairavan Lakshmanan<sup>2</sup>; Dasaradhi Palakodeti<sup>2</sup>; <sup>1</sup>Metabolomics Facility, C-CAMP, NCBS, Bangalore, India; <sup>2</sup>inSTEM, NCBS, Bangalore, India
- MP 399 **Combined Targeted Quantitation of Keto- and Amino Acids in GC-MS Analysis using MTBSTFA Derivatization;** Mimi Doll; Benjamin Wancewicz; Carol Tran; Mine Palazoglu; Oliver Fiehn; <sup>1</sup>NIH West Coast Metabolomics Center, UC Davis, Davis, CA
- MP 400 **Liquid Chromatography Mass Spectrometric Quantification of Immunomodulatory Histidine Metabolites of Probiotic *Lactobacillus reuteri* Strains;** Daniel Roeth<sup>1</sup>; Christina N. Morra<sup>2</sup>; James Versalovic<sup>2</sup>; Gabriel Gugiu<sup>1</sup>; Markus Kalkum<sup>1</sup>; <sup>1</sup>Department of Immunology, City of Hope, Duarte, CA; <sup>2</sup>Texas Children's Hospital, Baylor College, Houston, TX
- MP 401 **Improved Performance of Targeted Metabolome Analysis with Waters Xevo® TQ-S and Xevo® TQ-S Micro Instruments;** Ines Zitturi<sup>1</sup>; Christian Wachsmuth<sup>1</sup>; Harold Zott<sup>1</sup>; Michael Daxböck<sup>1</sup>; Cornelia Röhring<sup>1</sup>; Therese Koal<sup>1</sup>; Andrew Peck<sup>2</sup>; <sup>1</sup>Biocrates Life Science AG, Innsbruck, Austria; <sup>2</sup>Waters Corporation, Milford, MA
- MP 402 **Rapid Measurement of 8-oxo-7,8-dihydro-2'-deoxyguanosine in Urine of Colorectal Cancer Patients using Ultraperformance Liquid Chromatography–Tandem Mass Spectrometry;** Cheng Guo; Shu Zheng; <sup>1</sup>Zhejiang University, Hangzhou, China
- MP 403 **Determination of Metabolites in Plasma or Blood Using Parallel Ion-Exchange Column-Switching and Reversed-Phase UHPLC-MS/MS with Fast Polarity Switching;** Kyoko Watanabe<sup>1,2</sup>; Emmanuel Varesio<sup>1</sup>; Neil J Loftus<sup>3</sup>; Gérard Hopfgartner<sup>1</sup>; <sup>1</sup>University of Geneva, Geneva, Switzerland; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan; <sup>3</sup>Shimadzu MS/BU, Manchester, UK
- MP 404 **Simultaneous Stable Isotope Dilution Targeted and Untargeted Steroid Analysis with Girard P Derivatization on a QExactive High Resolution Mass Spectrometer;** Alexander Frey; Nathaniel Snyder; <sup>1</sup>AJ Drexel Autism Institute, Philadelphia, PA
- MP 405 **The Use of Capillary Electrophoresis Coupled to Mass Spectrometry (CESI-MS) for Quantitation of Nucleotides and Nucleosides with Minimal Sample Preparation;** Jose-Luis Gallegos-Perez; <sup>1</sup>Sciex, Framingham, MA

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- MP 406 **MET-COFEA + MET-XAlign: Tools that Enable LC/MS-based Comparative Metabolomics;** Wenchao Zhang; Patrick Xuechun Zhao; <sup>1</sup>Samuel Roberts Noble Foundation, Ardmore, OK
- MP 407 **Software for High-Throughput, Accurate Quantification of Mass Isotopomer Distributions from LC-MS Data for Metabolic Flux Analysis;** Yaroslav Lyutvinskiy<sup>1</sup>; Mohit Jain<sup>2</sup>; Roland Nilsson<sup>1</sup>; <sup>1</sup>Karolinska Institutet, Dept. of Medicine, Stockholm, Sweden; <sup>2</sup>UCSD, Dept. of Pharmacology, La Jolla, CA
- MP 408 **GNPS: Charting Molecular Families and Structure over Tens of Thousands of Mass Spectrometry Runs;** Mingxun Wang<sup>1</sup>; Haixu Tang<sup>2</sup>; Pieter Dorrestein<sup>3</sup>; Nuno Bandeira<sup>4</sup>; <sup>1</sup>UCSD, La Jolla, CA; <sup>2</sup>Indiana University, Bloomington, IN; <sup>3</sup>University of California, San Diego, Skaggs school, La Jolla, CA; <sup>4</sup>University of California, San Diego, La Jolla, CA
- MP 409 **METASPACE: A New European Project on Bioinformatics for Spatial Metabolomics;** Theodore Alexandrov<sup>1</sup>; Pieter Dorrestein<sup>2</sup>; Lennart Martens<sup>3</sup>; Oliver Panzer<sup>4</sup>; Charles Pineau<sup>5</sup>; Christoph Steinbeck<sup>6</sup>; Zoltan Takats<sup>7</sup>; Dennis Trede<sup>8</sup>; Kirill Veselkov<sup>7</sup>; <sup>1</sup>EMBL, Heidelberg, Germany; <sup>2</sup>University of California, San Diego, Skaggs school, La Jolla, CA; <sup>3</sup>VIB, Ghent, Belgium; <sup>4</sup>European Research Services GmbH, Muenster, Germany; <sup>5</sup>University of Rennes 1, Rennes, France; <sup>6</sup>EMBL-EBI, Hinxton, UK; <sup>7</sup>Imperial College London, London, N/A; <sup>8</sup>SCiLS GmbH, Bremen, Germany





- MP 410 **Investigation of Complex Isotope Patterns of <sup>13</sup>C-labeled Plant Metabolites by Mass Spectral Deconvolution;** Zhenzhen Wang<sup>1</sup>; [A. Daniel Jones](#)<sup>1</sup>; Yongdong Wang<sup>2</sup>; Ming Gu<sup>2</sup>; <sup>1</sup>Michigan State University, East Lansing, MI; <sup>2</sup>Cerno Bioscience, Norwalk, CT
- MP 411 **Maximizing GC-MS Metabolic Profiling Power using Both Targeted and Non-Targeted Analyses;** [Jinshu Qiu](#); Matt Jerums; Pik Kay Chan; Pavel Bondarenko; *Amgen, Thousand Oaks, CA*
- MP 412 **Metabolomics Analysis Operations Available for the BioCyc Pathway Database and Website;** Peter Karp; *Sri International, Menlo Park, CA*
- MP 413 **Development of Spectral Libraries for Use in Identification and Confirmation of Bourbon Authenticity;** [William Long](#)<sup>1</sup>; Luke Adams<sup>2</sup>; Sue D'Antonio<sup>1</sup>; <sup>1</sup>Agilent, Technologies, Little Falls, DE; <sup>2</sup>Beam Suntory, Louisville, KY
- MP 414 **Recent Advances in Skyline: Small Molecule Targets and Ion Mobility Filtering;** [Brian Pratt](#)<sup>1</sup>; Max Horowitz-Gelb<sup>1</sup>; J. Will Thompson<sup>2</sup>; Erin Baker<sup>3</sup>; Michael J. Maccoss<sup>1</sup>; Brendan Maclean<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Duke University School of Medicine, Durham, NC; <sup>3</sup>Pacific Northwest National Laboratory, Richland, WA
- MP 415 **New approach for Metabolomics Pathway Analysis;** [Takehiro Oshida](#)<sup>1</sup>; Teppei Ogawa<sup>1</sup>; Yasuto Yokoi<sup>1</sup>; Yukihiko Fukamachi<sup>1</sup>; Michihiro Araki<sup>2</sup>; Hiroki Makiguchi<sup>1</sup>; <sup>1</sup>Mitsui Knowledge Industry Co., Ltd., Minato-Ku, Japan; <sup>2</sup>Kobe University, Hyogo, Japan
- MP 416 **Disparate Metabolomics Data Reassembler: A Novel Algorithm for Agglomerating Incongruent LC-MS Metabolomics Datasets;** [Tytus Mak](#); Stephen Stein; *NIST, Gaithersburg, MD*
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- MP 418 **A Novel Method for Theoretically Determining the Success Rate of Identification by MS<sup>1</sup> Using a Human Metabolome Database;** [Scott Walmsley](#); Nichole Reisdorph; *National Jewish Health, Denver, CO*
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- MP 419 **Masses and Expected Compounds: Automatic Creation of Context-Specific Databases and Tripartite Identification of Substances using SpiderMass;** Robert Winkler; *CINVESTAV Unidad Irapuato, Irapuato, Mexico*
- MP 420 **Stochastic Modeling of Proteome Turnover from Stable Isotope Labeling and LC-MS;** Ling Li<sup>2</sup>; Belinda Willard<sup>2</sup>; Tahir Kasumov<sup>2</sup>; [Rovshan Sadygov](#)<sup>1</sup>; <sup>1</sup>University of Texas, Galveston, TX; <sup>2</sup>Cleveland Clinic, Cleveland, OH
- MP 421 **A Logical Bayesian Framework to Dynamically Compose a Modular Inductive Model of a Proteomics Experiment;** [Kurt De Grave](#); Jan Ramon; *KU Leuven, Leuven, Belgium*
- MP 422 **Assigning Confidence to Peptide Spectrum Matches Based on Permutation Analysis;** Brian Mitchell; Anoop Mayampurath; Stephen Kron; [Samuel Volchenbom](#); *University of Chicago, Chicago, IL*
- MP 423 **Ranking Chemical Formulas by Isotopic Pattern Recognition;** Stephen E. Reichenbach<sup>1</sup>; [Mehrdad Zaker Shahrak](#)<sup>1</sup>; Qingping Tao<sup>2</sup>; <sup>1</sup>University of Nebraska - Lincoln, Lincoln, NE; <sup>2</sup>GC Image, LLC, Lincoln, NE
- MP 424 **Towards the Development of a Factor Analysis Based Alignment Algorithm for Raw GC-TOFMS Data;** Peter Willis; Elizabeth Humston-Fulmer; Jihong Wang; [Sandy Liu](#); *LECO Corp, St. Joseph, MI*
- MP 425 **Mathematical Qualimetry for Mass Spectrometry: Optimization and Harmonization of Sample Preparation, Data Processing and Data Mining;** Alexander Bolkhovitinov; *IMS, New York, NY*
- MP 426 **Analysis of Unexplained Peaks and Corresponding Relationship Patterns in MS/MS Spectra;** [Aida Mrzic](#)<sup>1</sup>; Wout Bittremieux<sup>1</sup>; Trung Nghia Vu<sup>3</sup>; Dirk Valkenborg<sup>2</sup>; Kris Laukens<sup>1</sup>; <sup>1</sup>University of Antwerp, Antwerpen, Belgium; <sup>2</sup>VITO Mol, Antwerpen, Belgium; <sup>3</sup>Karolinska Institutet, Stockholm, Sweden
- MP 427 **Advancing Computer-Assisted Structure Elucidation Methods: A Large-Scale Fragment Assignment Project using Heuristic and Molecular Modeling Methods;** Michal Raab; Juraj Lutisan; [Robert Mistrik](#); *HighChem, Bratislava, Slovakia*
- MP 428 **A Method for Automated Data Extraction and Peak Identification from Large GC-MS Data Sets Using Multivariate Analysis;** [Joshua Coon](#); Mark Van Benthem; James Hochrein; Curtis Mowry; *Sandia National Laboratories, Albuquerque, NM*
- MP 429 **Targeted and Untargeted Feature Extraction for GC/MS Spectral Data Profiling;** [Norton Kitagawa](#); Anthony Gray; Jennifer Gushue; Stephen Madden; Yinghang Yang; *Agilent Technologies, Inc., Santa Clara, CA*
- MP 430 **A Probabilistic Iterative Algorithm for Unrestrictive Protein Modification Localization;** [Zhiwu An](#)<sup>1</sup>; Yan Fu<sup>1</sup>; Wantao Ying<sup>2</sup>; Xiaohong Qian<sup>2</sup>; Fuzhou Gong<sup>1</sup>; <sup>1</sup>Academy of Mathematics and Systems Science, CAS, Beijing, China; <sup>2</sup>Beijing Proteome Research Center, Beijing, China
- MP 431 **An Algorithm for Generating a Representative Protein Sequence Database to Facilitate Proteomic Analysis of Unsequenced Organisms;** [Marlon Dias Mariano Dos Santos](#)<sup>1</sup>; Juliana de Saldanha da Gama Fischer<sup>1</sup>; Felipe da Veiga Leprvost<sup>1</sup>; Valmir C. Barbosa<sup>2</sup>; Paulo Costa Carvalho<sup>1</sup>; <sup>1</sup>Laboratory for Proteomics and Protein Engineering, Curitiba, Brazil; <sup>2</sup>Systems Engineering and Computer Science Program, Rio de Janeiro, Brazil
- MP 432 **Computational Platform for the Comprehensive Analysis of Clinical Proteomic Data;** [Stefka Tyanova](#)<sup>1</sup>; Tikira Temu<sup>1</sup>; Arthur Carlson<sup>1</sup>; Pavel Sinitcyn<sup>1</sup>; Sally Deeb<sup>1</sup>; Tamar Geiger<sup>2</sup>; Matthias Mann<sup>1</sup>; Juergen Cox<sup>1</sup>; <sup>1</sup>Max Planck Institute of Biochemistry, Martinsried, Germany; <sup>2</sup>Sackler Faculty of Medicine, Tel Aviv University, Tel Aviv, Israel
- MP 433 **Concordance of Peptide Assignments between Different Search Engines;** Fatemeh Ghavidel<sup>3</sup>; Wout Bittremieux<sup>2</sup>; Kris Laukens<sup>2</sup>; Tomasz Burzykowski<sup>3</sup>; [Dirk Valkenborg](#)<sup>1</sup>; <sup>1</sup>VITO, Mol, Belgium; <sup>2</sup>University of Antwerp, Antwerp, Belgium; <sup>3</sup>Hasselt University, Hasselt, Belgium
- MP 434 **Processing of 3D Imaging Hyperspectral Datasets for Explorative Analysis of Tumour Heterogeneity;** [James Mckenzie](#); Nicole Strittmatter; Anna Mróz; Zoltan Takats; Kirill Veselkov; *Imperial College, London, UK*
- MP 435 **Identifying Targeted Compounds in Un-Supervised Ion Clusters Using Advance Proteome Modeling;** [Keith Fadgen](#); Steve Ciavarini; Scott Geromanos; *Waters Corporation, Milford, MA*
- MP 436 **The Problem of Polydispersity: Tackling Complex Spectra with a Bayesian Approach;** [Michael Marty](#); Carol Robinson; *University of Oxford, Oxford, Oxfordshire*
- MP 437 **Signature of Life in terrestrial mass distribution of C, H, N and O;** [Roman Zubarev](#)<sup>2</sup>; Alexander Zubarev<sup>1</sup>; <sup>1</sup>EXNA AB, Stockholm, Sweden; <sup>2</sup>Karolinska Institute, Stockholm, Sweden
- MP 438 **Proteome Characterization by top-Down Tandem Mass Spectra;** Qiang Kou<sup>1</sup>; Binhai Zhu<sup>2</sup>; [Xiaowen Liu](#)<sup>1,3</sup>; <sup>1</sup>Indiana University Purdue University Indianapolis, Indianapolis, IN; <sup>2</sup>Montana State University, Bozeman, MT; <sup>3</sup>Indiana University School of Medicine, Indianapolis, IN
- MP 439 **Novor: Real-Time Peptide de Novo Sequencing;** Bin Ma; *University of Waterloo, Waterloo, Canada*

- MP 440 **Nonconvex Quasi-Norm-Based Normalization of MALDI MSI Data**; Luis Mancera<sup>1</sup>; Philippa Hart<sup>1</sup>; Fiona Henderson<sup>2</sup>; Hervé Boutin<sup>2</sup>; Adam McMahon<sup>2</sup>; Omar Belgacem<sup>1</sup>; <sup>1</sup>Shimadzu, Kratos, Manchester, UK; <sup>2</sup>Wolfson Molecular Imaging Centre, Manchester, UK
- MP 441 **De novo Identification of Small Molecules Using an Excel Add In**; Daniel L. Sweeney; MathSpec, Inc., Arlington Heights, IL
- MP 442 **Bioinformatics for Mass Spectrometry Imaging in Augmented Systems Histology**; Kirill Veselkov; James McKenzie; Ottmar Golf; Nicole Strittmatter; Reza Mirnezami; James Kinross; Ara Darzi; Elaine Holmes; Jeremy Nicholson; Zoltan Takats; Imperial College, London, London
- MP 443 **Validating and Comparing Component Detection Algorithms for LC-MS data**; Jane Razumovskaya; Joseph Brown; David Wright; Richard Baran; Iman Mohtashemi; Thermo Fisher Scientific, San Jose, CA
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- MP 444 **Combined Rat Serum Lipidomics and Brain Multimodal MS Imaging for the Detection of Mild Traumatic Brain Injury**; Scott Hogan; Rachel Bennett; Christina Jones; David Gaul; Melissa Alvarado-Valez; Michlle LaPlaca; Facundo Fernandez; Georgia Institute of Technology, Atlanta, GA
- MP 445 **A Mass Spectrometry Proteomics Based Approach for Differentiating Thoracic Tumor Subtypes**; Linan Wang<sup>1,2</sup>; Konstantin Shilo<sup>1,3</sup>; Charles Hitchcock<sup>1,3</sup>; Michael A. Freitas<sup>1,2</sup>; <sup>1</sup>Ohio State University, Columbus, OH; <sup>2</sup>Department of Molecular Virology, Immunology and M, Columbus, OH; <sup>3</sup>Department of Pathology, Columbus, OH
- MP 446 **Detection of FGF15 in Plasma by Stable Isotope Standard Capture with Anti-Peptide Antibodies and Targeted Mass Spectrometry**; Hamid Mirzaei<sup>1</sup>; David Mangelsdorf<sup>1</sup>; Steven Kliwer<sup>1</sup>; Andrew Lemoff<sup>1</sup>; Takeshi Katafuchi<sup>1</sup>; Daria Esterhazy<sup>2</sup>; Xunshan Ding<sup>3</sup>; <sup>1</sup>University of Texas Southwestern, Dallas, TX; <sup>2</sup>Rockefeller University, New York, NY; <sup>3</sup>NGM Biopharmaceuticals, Inc., San Francisco, CA
- MP 447 **Receiver Operating Characteristic Analysis of Identified and Un-Identified Peptides using Label-Free Quantification in MaxQuant**; Jana M. Rucker; Lindsay Schambeau; Lewis K. Pannell; Mitchell Cancer Institute, Mobile, AL
- MP 448 **Application of TMTcalibrator+ for Detection of Markers of Microglia Activation in CSF of Alzheimer's Disease Patients**; Claire Russell<sup>1</sup>; Vikram Mitra<sup>1</sup>; Amanda Heslegrave<sup>2</sup>; Jennifer Pocock<sup>2</sup>; Henrik Zetterberg<sup>3</sup>; Ian Pike<sup>1</sup>; Malcolm Ward<sup>1</sup>; <sup>1</sup>Proteome Sciences plc, London, UK; <sup>2</sup>Institute of Neurology, University College London, London, UK; <sup>3</sup>University of Gothenburg, Gothenburg, Sweden
- MP 449 **N- and O-glycomics from Formalin-Fixed Paraffin-Embedded (FFPE) Clinical Specimens using Porous Graphitized Carbon LC-ESI IT-MS/MS**; Hannes Hinneburg<sup>1,2</sup>; Petra Korac<sup>3</sup>; Slavko Gasparov<sup>4,5</sup>; Peter H. Seeberger<sup>1,2</sup>; Vlatka Zoldo<sup>3</sup>; Daniel Kolarich<sup>1</sup>; <sup>1</sup>MPI of Colloids and Interfaces, Potsdam, Germany; <sup>2</sup>Free University Berlin, Berlin, Germany; <sup>3</sup>Dept. of Biology, University of Zagreb, Zagreb, Croatia; <sup>4</sup>Inst. for Path. and Cytology, Uni Hospital Merkur, Zagreb, Croatia; <sup>5</sup>Department of Pathology, Medical School Zagreb, Zagreb, Croatia
- MP 450 **High Resolution Shotgun Proteomic Analysis for Biomarker Discovery of Occupational and Environmental Nanoparticles Exposure**; Nesperin Ali<sup>1</sup>; Stefan Ljunggren<sup>2</sup>; Helen M Karlsson<sup>2</sup>; Jörn Nielsen<sup>1</sup>; Anders Gudmundsson<sup>1</sup>; Christian H Lindh<sup>1</sup>; Bo AG Jönsson<sup>1</sup>; Monica Käredal<sup>1</sup>; <sup>1</sup>Lund University, Lund, Sweden; <sup>2</sup>Linköping University, Linköping, Sweden
- MP 451 **The Differentiation of Orexin Receptor Antagonists and GABA Agonists on Brain Acetylcholine and Histamine Using In Vivo Microdialysis and LC/MS**; Lihang Yao; Andres Ramirez; Anthony Gotter; Anthony Roecker; Steven Fox; Jason Uslaner; Paul Coleman; Christopher Winrow; Sean Smith; John Renger; Merck, Co; Inc, West Point, PA
- MP 452 **Characterization and Quantitative Comparison of the Adult and Pediatric Urinary Glycomes by LC-MS To Develop a Baseline Standard**; Patricia Cho; Hui Zhou; Stephen Kostel; John Froehlich; Richard Lee; Boston Children's Hospital, Harvard Medical School, Boston, MA
- MP 453 **Genome-Scale Proteomic Profiling Identifies Breast Cancer Progression Markers**; Yair Pozniak<sup>1</sup>; Iris Barshack<sup>2</sup>; Tamar Geiger<sup>1</sup>; <sup>1</sup>Tel Aviv University, Tel Aviv, Israel; <sup>2</sup>Sheba Medical Center, Ramat Gan, IL
- MP 454 **Identification of a Protein Substrate Specific for Histone Deacetylase 11 (HDAC11)**; Uwe Warnken<sup>1</sup>; Marie Catherine Schier<sup>1</sup>; Ramona Mayer<sup>1</sup>; Hedwig Deubzer<sup>2</sup>; Olaf Witt<sup>3</sup>; Martina Schnölzer<sup>1</sup>; <sup>1</sup>German Cancer Research Center, Heidelberg, Germany; <sup>2</sup>Charité, Dept. of Pediatric Oncology, Berlin, Germany; <sup>3</sup>University Hospital, Dept. of Pediatric Oncology, Heidelberg, Germany
- MP 455 **Development of PEP Technology for Biomarker Discoveries and Functional Proteomics Studies**; Xing Wang; Michael Davies; Array Bridge Inc., St. Louis, Missouri
- MP 456 **Proteomic Imaging for Brain and Spinal Cord from Experimental Allergic Encephalomyelitis (EAE) Mouse Model**; Takashi Nirasawa<sup>1</sup>; Noriyuki Iwasaki<sup>1</sup>; Takayuki Kondo<sup>2</sup>; Akimitsu Miyake<sup>3</sup>; Hiroki Yamashita<sup>3</sup>; Masaya Ikegawa<sup>3</sup>; <sup>1</sup>Bruker Daltonics K.K., Yokohama, Japan; <sup>2</sup>Kyoto University, Kyoto, Japan; <sup>3</sup>Doshisha University, Kyoto, Japan
- MP 457 **Identification of Biomarkers of Dermal Exposure to Toluene Diisocyanate**; Justin M. Hettick; Ajay P. Nayak; Paul D. Siegel; NIOSH, Morgantown, WV
- MP 458 **GC-MS Based Metabolic Analysis of Plasma for Biomarker Discovery**; Cristina Di Poto; Alessia Ferrarini; Yue Luo; Mohammad R. Nezami Ranjbar; Rency Varghese; Chi Zhang; Habtom Resson; Georgetown University, Lombardi Cancer Center, Washington, DC
- MP 459 **Application of TMTcalibrator+ and Phosphopeptide Enrichment for Global Phosphoproteomic Analysis of CSF from Alzheimer's Disease Patients**; Claire Russell; Vikram Mitra; Ian Pike; Malcolm Ward; Proteome Sciences plc, London, UK
- MP 460 **The Use of Exhaled Breath for the Identification of Hypoxia Biomarkers**; Sean Harshman<sup>1</sup>; Brian Geier<sup>1</sup>; Maomian Fan<sup>1</sup>; Sage Rinehardt<sup>1</sup>; Brandy Watts<sup>1</sup>; Leslie Drummond<sup>2</sup>; George Preti<sup>3</sup>; Jeffrey Phillips<sup>2</sup>; Darrin Ott<sup>1</sup>; Claude Grigsby<sup>1</sup>; <sup>1</sup>Air Force Research Laboratory, WPAFB, OH; <sup>2</sup>Naval Medical Research Unit-Dayton, WPAFB, OH; <sup>3</sup>Monell Chemical Senses Center, Philadelphia, PA
- MP 461 **IgG Glycosylation as a Biomarker for Pancreatic Diseases**; Hsi-Chang Shih<sup>1,3</sup>; Ming-Chu Chang<sup>2</sup>; Chein-Hung Chen<sup>3</sup>; Ya-Po Kuo<sup>3</sup>; Chung-Hsuan Chen<sup>1,3</sup>; Yu-Ting Chang<sup>2</sup>; <sup>1</sup>Dept. of Chemistry, National Taiwan University, Taipei, Taiwan; <sup>2</sup>Dept. of Internal Medicine, NTU Hospital, Taipei, Taiwan; <sup>3</sup>The Genomics Research Center, Academia Sinica, Taipei, Taiwan
- MP 462 **A Sensitive and Versatile Analytical Method for Quantification of Cyclic Nucleotide Monophosphates (cNMPs) in Biological Systems: Application to Novel Biomarkers**; Xin Jia; Emily Weinert; Emory University, Decatur, Georgia



- MP 463 **Detection and Confirmation of Novel Serum Lipid Biomarkers Predicting Preeclampsia using a Shotgun Lipidomics Approach;** Swati Anand<sup>1</sup>; Sydney Young<sup>1</sup>; Sean Esplin<sup>2</sup>; Bruce Jackson<sup>1</sup>; Dennis H. Tolley<sup>1</sup>; Steven W. Graves<sup>1</sup>; <sup>1</sup>BYU, Provo, UT; <sup>2</sup>University of Utah School of Medicine, Salt Lake City, UT
- MP 464 **Cross-Site Identification of Ovarian Cancer Proteomic Biomarkers from Cervicovaginal Fluid;** Lindsay Schambeau<sup>1</sup>; Brian Hood<sup>2</sup>; Thomas Conrads<sup>2</sup>; Michael Finan<sup>1</sup>; Rodney Rocconi<sup>1</sup>; Laurie Owen<sup>1</sup>; Michael Chambers<sup>3</sup>; Jana Rucker<sup>1</sup>; Lewis Pannell<sup>1</sup>; <sup>1</sup>Mitchell Cancer Institute, Mobile, AL; <sup>2</sup>Women's Health Integrated Research Center, Annandale, VA; <sup>3</sup>Swift Biotechnology LLC, Mobile, AL
- MP 465 **Radiation Exposure Induces Alterations Typical of Oxidative Stress Modifications Underlying Cardiovascular Disease;** Mark E. McComb<sup>1</sup>; Markus M. Bachschmid<sup>1</sup>; Chunxiang Yao<sup>1</sup>; Maggie Kuo<sup>2</sup>; Stephen Whelan<sup>1</sup>; Jean Spencer<sup>1</sup>; Christian Heckendorf<sup>1</sup>; Catherine E. Costello<sup>1</sup>; Dan Berkowitz<sup>2</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA; <sup>2</sup>Johns Hopkins University, Baltimore, MD
- MP 466 **The Investigation of Extraction Efficiency of Proteins from Brain Tissues Related to Alzheimer's Disease;** Siddhita Aparaj-Shirsat; Rachel Marvin; Kenneth Hensley; Dragan Isailovic; *University of Toledo, Toledo, OH*
- BIOMARKERS: QUANTITATIVE ANALYSIS (PROTEIN)**  
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- MP 467 **SI-Traceable Quantification of 1-32 Brain Natriuretic Peptide in Plasma at Clinically Relevant Concentration Levels;** Frank Attila Torma<sup>1,2</sup>; Kate Groves<sup>1</sup>; Sabine Biesenbruch<sup>1</sup>; Christopher Mussell<sup>1</sup>; Rainer Cramer<sup>2</sup>; Milena Quaglia<sup>1</sup>; <sup>1</sup>LGC LTD, Teddington, UK; <sup>2</sup>University of Reading, Reading, UK
- MP 468 **Multiplexed Protein Quantification of Salivary Proteins by MRM-MS for Evaluation of Cancer Biomarkers;** Yi-Ting Chen<sup>1</sup>; Hsiao-Wei Chen<sup>1</sup>; Wei-Fan Chiang<sup>2</sup>; Jau-Song Yu<sup>1</sup>; Yu-Sun Chang<sup>1</sup>; Chun-Feng Wu<sup>1</sup>; <sup>1</sup>Chang Gung University, Taoyuan, Taiwan; <sup>2</sup>Chi-Mei Medical Center, Liouying, Taiwan
- MP 469 **Detection and Quantification of Relevant Proteins in GBM FFPE Tumor Tissue Using Selective Reaction Monitoring Mass Spectrometry;** Xiaolin Li<sup>1</sup>; Jill Barnholtz-Sloan<sup>1,2</sup>; Daniela M Schlatter<sup>1</sup>; Mark Chance<sup>1</sup>; <sup>1</sup>Case Western Reserve University, Cleveland, OH; <sup>2</sup>Comprehensive Cancer Center University Hospitals, Cleveland, OH
- MP 470 **Development of the Workflow for targeted Proteomic Quantification of Osteopontin in Healthy and Cancerous Human Breast Tissues;** Katarzyna Macur<sup>1</sup>; Lars Hagen<sup>2</sup>; Tomasz Ciesielski<sup>2</sup>; <sup>1</sup>Intercollegiate Faculty of Biotechnology UG-MUG, Gdansk, Poland; <sup>2</sup>Norwegian University of Science and Technology, Trondheim, Norway
- MP 471 **First Quantification of Human CSF Tau Protein without Immunocapture using Triple Quadrupole Mass Spectrometer;** Christophe Hirtz<sup>1</sup>; Pauline Bros<sup>1</sup>; Nicolas Barthelemy<sup>1</sup>; Vincent Delatour<sup>3</sup>; Jérôme Vialaret<sup>1</sup>; Audrey Gabelle<sup>2</sup>; Sylvain Lehmann<sup>1</sup>; <sup>1</sup>LBPC-IRB, CHU de Montpellier, Montpellier, France; <sup>2</sup>Centre Mémoire Ressources Recherche, Montpellier, France; <sup>3</sup>Laboratoire National de Métrologie et d'Essais, Paris, France
- MP 472 **Core-fucosylated Glycopeptides in Hepatocellular Carcinoma;** Haidi Yin<sup>1</sup>; Zhijing Tan<sup>1</sup>; Jing Wu<sup>1</sup>; Jianhui Zhu<sup>1</sup>; Jorge Marrero<sup>2</sup>; David Lubman<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>University of Texas, Dallas, TX
- MP 473 **PTM Profiling of Cancer Cells by Sequential Enrichment for Methylation, Acetylation and Phosphorylation to Monitor Cellular Signaling Upon Adenosine-2',3'-Dialdehyde Treatment;** Ghaith Hamza<sup>2</sup>; Charles Farnsworth<sup>1</sup>; Hongbo Gu<sup>1</sup>; Xiaoying Jia<sup>1</sup>; Jeffrey Silva<sup>1</sup>; <sup>1</sup>Cell Signaling Technology, Danvers, MA; <sup>2</sup>Endicott College, Beverly, MA
- MP 474 **Target Analysis of Prostate-Specific Antigen Glycopeptide Abundance in Prostate Cancer and Benign Hyperplasia from Urinary Samples;** Chun-Jen Hsiao<sup>1,2</sup>; Tzong-Shin Tzai<sup>3</sup>; Chein-Hung Chen<sup>1</sup>; Wen-Horn Yang<sup>3</sup>; Chung-Hsuan Chen<sup>1</sup>; <sup>1</sup>Academia Sinica, Taipei, Taiwan; <sup>2</sup>National Yang-Ming University, Taipei, Taiwan; <sup>3</sup>National Chen Kung University Hospital, Tainan, Taiwan
- MP 475 **Quantification of Human IL-6 in Serum with an Automated Online Sample Preparation System Coupled with LC-MS;** Li Li<sup>1</sup>; Nishi Rochelle<sup>2</sup>; Hiralben Patel<sup>1</sup>; Kevin Schug<sup>1</sup>; Joe Barrera<sup>1</sup>; <sup>1</sup>University of Texas at Arlington, Arlington, TX; <sup>2</sup>Shimadzu Scientific Instruments, Inc, Addison, IL
- MP 476 **Protein-based Biomarker Predicts Conversion from Clinically Isolated Syndrome to Multiple Sclerosis;** Eva Borràs<sup>1,2</sup>; Ester Cantó<sup>3</sup>; Meena Choi<sup>4</sup>; Luisa María Villar<sup>5</sup>; Jose Carlos Álvarez-Cermeño<sup>5</sup>; Cristina Chiva<sup>2</sup>; Xavier Montalbán<sup>3</sup>; Olga Vitek<sup>4</sup>; Manuel Comabella<sup>3</sup>; Eduard Sabidó<sup>1,2</sup>; <sup>1</sup>Proteomics Unit (CRG), Barcelona, Spain; <sup>2</sup>University Pompeu Fabra (UPF), Barcelona, Spain; <sup>3</sup>Cemcat. Institut de Recerca Vall Hebrón, Barcelona, Spain; <sup>4</sup>Department of Statistics, Purdue University, West Lafayette, IN; <sup>5</sup>Hospital Ramón y Cajal, Madrid, Spain
- MP 477 **Validation of LRG1 as a Potential Biomarker for Detection of Epithelial Ovarian Cancer by a Blinded Study;** Jing Wu; Haidi Yin; Jianhui Zhu; Ronald Buckanovich; David Lubman; *University of Michigan, Ann Arbor, MI*
- MP 478 **Human Cerebrospinal Fluid and Surrogate Matrix-Based Quantification of Alzheimer's Biomarker Amyloid Beta Protein by Liquid Chromatography-Tandem Mass Spectrometry;** Mei Chen<sup>1</sup>; Weiming Xia<sup>2</sup>; <sup>1</sup>Harvard School of Public Health, Boston, MA; <sup>2</sup>ENR Memorial VA Hospital, Bedford, MA
- MP 479 **Comparative Two Dimensional Polyacrylamide Gel Electrophoresis (2D-PAGE) of the Salivary Proteome of Children with Autism Spectrum Disorder (ASD);** Armand Ngounou<sup>1</sup>; Kelly L. Wormwood<sup>1</sup>; Laci Charette<sup>2</sup>; Jeanne P. Ryan<sup>3</sup>; Alisa G. Woods<sup>1</sup>; Costel C. Darie<sup>1</sup>; <sup>1</sup>Clarkson University, Potsdam, NY; <sup>2</sup>SUNY Plattsburgh Neuropsychology Clinic, Plattsburgh, NY; <sup>3</sup>Department of Psychology, SUNY Plattsburgh, Plattsburgh, NY
- MP 480 **LC-MS/MS Quantification of Factor P (Properdin), an Endogenous Protein, in Monkey Serum;** Xinliu Gao; Hui Lin; Wenkui Li; Jimmy Flarakos; Francis Tse; *Novartis Institutes for Biomedical Research, East Hanover, NJ*
- MP 481 **Quantitation of N-terminal Formaldehyde Adducts to Hemoglobin using UPLC-MS/MS;** Min Yang<sup>1</sup>; Chui Tse<sup>2</sup>; Maria Ospina<sup>2</sup>; Hubert Vesper<sup>2</sup>; <sup>1</sup>Battelle Memorial Institute, Atlanta, GA; <sup>2</sup>Centers for Disease Control and Prevention, Atlanta, GA
- MP 482 **Quantitation of Calcyclin and Heat Shock Protein 90 in Serum from Preeclampsia Patients by 2D Nano LC-MS/MS;** Coşkun Güzel<sup>1</sup>; Caroline B. van den Berg<sup>1</sup>; Régine P.M. Steegers-Theunissen<sup>1</sup>; Lennard Dekker<sup>1</sup>; Johannes P.C. Vissers<sup>2</sup>; Eric A.M. Steegers<sup>1</sup>; Theo M. Luidert<sup>1</sup>; <sup>1</sup>Erasmus Medical Center, Rotterdam, Netherlands; <sup>2</sup>Waters Corporation, Manchester, UK
- MP 483 **Measuring Acute Traumatic Brain Injury Biomarkers by Targeted Mass Spectrometry;** Sean Shen<sup>1</sup>; Ina-Beate Wanner<sup>2</sup>; Joseph A. Loo<sup>1</sup>; <sup>1</sup>Chemistry & Biochemistry, University of California, Los Angeles, CA; <sup>2</sup>Semel Institute for Neuroscience & Human Behavior, University of California, Los Angeles, CA



## MONDAY POSTERS

- MP 484 **Detection and Relative Quantitation of Potential Salivary Antimicrobial Biomarkers (HNP 1-4) by LC-ESI-MS in Young Athletes;** N. Ashrafi; F.S. Pullen; B.V. Nielsen; *University of Greenwich, Chatham Maritime, UK*
- MP 485 **Western Diet Alters O-GlcNAcylation and Phosphorylation in Mouse Heart Metabolic Disorder;** Stephen A. Whelan<sup>1</sup>; Jean Spencer<sup>1</sup>; Christian Heckendorf<sup>1</sup>; Junfeng Ma<sup>2</sup>; Chunxiang Yao<sup>1</sup>; Jessica Behring<sup>1</sup>; Deborah Siwick<sup>1</sup>; Wilson Colucci<sup>1</sup>; Richard Cohen<sup>1</sup>; Markus Bachschmid<sup>1</sup>; Gerald W. Hart<sup>2</sup>; Catherine E. Costello<sup>1</sup>; Mark E. Mccomb<sup>1</sup>; <sup>1</sup>*Boston University School of Medicine, Boston, MA*; <sup>2</sup>*Johns Hopkins University School of Medicine, Baltimore, MD*
- MP 486 **Application of nanoLC-MS/MS to Measure Glycated N-terminal Beta Hemoglobin in Bottlenose Dolphins;** Michael Janech<sup>1</sup>; Alison Bland<sup>1</sup>; Stephanie Venn-Watson<sup>2</sup>; <sup>1</sup>*Medical University of South Carolina, Charleston, SC*; <sup>2</sup>*The National Marine Mammal Foundation, San Diego, CA*
- MP 487 **Evaluation of Candidate Biomarkers for FGF-associated Breast Cancer by Selected Reaction Monitoring Mass Spectrometry;** Hongyan Zhao; Andrew Creese; Debbie Cunningham; John Heath; Helen Cooper; *School of Biosciences, University of Birmingham, Birmingham, UK*
- MP 488 **Quantitation of Bradykinin and Bradykinin 1-5 in Human Plasma Using a 2D-LC-MS/MS Assay with a Surrogate Analyte Approach;** Moucun Yuan<sup>1</sup>; Hongmei Cao<sup>2</sup>; Eric Ma<sup>1</sup>; William R. Mylott<sup>1</sup>; Bruce Hidy<sup>1</sup>; Rand Jenkins<sup>1</sup>; Jiang Wu<sup>2</sup>; Ann Gooding<sup>2</sup>; Yongchang Qiu<sup>2</sup>; <sup>1</sup>*PPD, Richmond, VA*; <sup>2</sup>*Shire, Lexington, MA*
- PLANT-OMICS**  
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- MP 489 **Investigation of Polyphenols in White and Coloured Flower Petals of Faba Bean Plants;** Yurdagul Ferhatoglu; Mahla Mirali; Randy W. Purves; Kirstin E. Bett; Albert Vandenberg; *University of Saskatchewan, Saskatoon, Canada*
- MP 490 **Identification of Cold-induced MAP Kinase Substrates in *Arabidopsis Thaliana* through Protein Kinase Assay Linked-Phosphoproteomics;** Chuan-Chih Hsu<sup>1</sup>; Chunzhao Zhao<sup>2</sup>; Pengcheng Wang<sup>2</sup>; Jian-Kang Zhu<sup>2</sup>; Weiguo Andy Tao<sup>1</sup>; <sup>1</sup>*Department of Biochemistry, Purdue University, West Lafayette, IN*; <sup>2</sup>*Department of Horticulture, Purdue University, West Lafayette, IN*
- MP 491 **Label-free Quantitative Analysis by WiSIM-DIA with an Orbitrap Fusion to Identify Proteins Involved in the Cuticle Formation of Tomato Fruit;** Laetitia Martin<sup>1</sup>; Joshua Nicklay<sup>2</sup>; Tara Schroeder<sup>2</sup>; Tahmid Hassan<sup>2</sup>; Elizabeth Anderson<sup>3</sup>; Jocelyn Rose<sup>1</sup>; Sheng Zhang<sup>3</sup>; <sup>1</sup>*School of Integrative Plant Science, Cornell Univ, Ithaca, NY*; <sup>2</sup>*Thermo Fisher Scientific, Somerset, NJ*; <sup>3</sup>*Proteomics & Mass Spec Facility, Cornell Univ, Ithaca, NY*
- MP 492 **Acetylome Analysis Reveals Lysine Acetylation is in Regulation of Photosynthesis and Carbon Metabolism in Cyanobacterium *Synechocystis*;** Ran Mo<sup>2</sup>; Mingkun Yang<sup>2</sup>; Zhongyi Cheng<sup>1</sup>; Xingling Yi<sup>1</sup>; Feng Ge<sup>2</sup>; <sup>1</sup>*PTM Biolabs, Inc, Hangzhou, China*; <sup>2</sup>*Chinese Academy of Sciences, Wuhan, CN*
- MP 493 **The Application of Capillary Electrospray Ionization with Negative Ion Electrospray Ionization to the Analysis of Plant Metabolites;** Stephen J. Lock<sup>1</sup>; Edna Betgovargez<sup>2</sup>; <sup>1</sup>*ABSCIEX, Warrington, UK*; <sup>2</sup>*Sciex Separations, Brea, CA*
- MP 494 **Determination of *in situ* Plant Root Metabolomes by Ambient Ionization Mass Spectrometry;** Rabi A. Musah<sup>1</sup>; Robert B. Cody<sup>2</sup>; Ashton D. Lesiak<sup>1</sup>; Max J. Maron<sup>1</sup>; David Edwards<sup>2</sup>; A. John Dane<sup>2</sup>; Michael C. Long<sup>1</sup>; <sup>1</sup>*University at Albany-SUNY, Albany, NY*; <sup>2</sup>*JEOL USA, Inc., Peabody, MA*
- MP 495 **Elucidation of Cellulosic Transcription Factors in Stem Differentiating Xylem Tissue of *Populus trichocarpa*;** Philip Loziuk; Jennifer Parker; Wei Li; Chien-Yuan Lin; Jack Wang; Quanzi Li; Ronald Sederoff; Vincent Chiang; David Muddiman; *North Carolina State University, Raleigh, NC*
- MP 496 **Pathogen-triggered Protein-Protein Interactions Mediating Nonclassical Secretion of Mannitol Dehydrogenase in Plants;** Tricia Ho; Kevin Blackburn; John Williamson; Michael Goshe; *North Carolina State University, Raleigh, NC*
- MP 497 **Analysis of Gape Xylem Tissue and Sap Proteome;** Ramesh Katam; Varshini Sridhar; Sydney Lyda; *Department of Biological Sciences, Florida A&M Univ, Tallahassee, FL*
- MP 498 **<sup>13</sup>C-amino Acid Labeling Investigation of Acylsugar Related Aliphatic Acid Elongation via UHPLC-QTOF-MS/MS Analysis;** Xiaoxiao Liu<sup>1</sup>; Banibrata Ghosh<sup>2</sup>; A. Daniel Jones<sup>1,2</sup>; <sup>1</sup>*Department of Chemistry, Michigan State University, East Lansing, MI*; <sup>2</sup>*Department of Biochemistry and Molecular Biology, Michigan State University, East Lansing, MI*
- MP 499 **Response of *Chlamydomonas reinhardtii* Proteome to Wastewater Culturing: A Comparative Label-Free Proteomic Analysis;** Anil K. Patel; Mark G. Lefsrud; *McGill University, Ste. Anne De Bellevue, Canada*
- MP 500 **Identification and Classification of *Salvia* Species using Ambient Ionization Mass Spectrometry;** Justine E. Giffen<sup>2</sup>; Ashton D. Lesiak<sup>2</sup>; Robert B. Cody<sup>1</sup>; Rabi Musah<sup>2</sup>; <sup>1</sup>*JEOL USA, Inc., Peabody, MA*; <sup>2</sup>*University at Albany-SUNY, Albany, NY*
- MP 501 **Mapping Phenolic Glycosides in *Populus deltoides* and *Populus grandidentata* by Leaf Spray Mass Spectrometry;** Dalton Snyder; Christina Schilling; Cris Hochwender; Arlen Kaufman; *University of Evansville, Evansville, IN*
- MP 502 **Comparative Proteomic Analysis of Two Rice Genotypes with Contrasting Drought Tolerance;** Mehdi Mirzaei<sup>1</sup>; Yunqi Wu<sup>1</sup>; Dana Pascovici<sup>2</sup>; Joel Chick<sup>3</sup>; Brian Atwell<sup>1</sup>; Paul Haynes<sup>1</sup>; <sup>1</sup>*Macquarie University, Sydney, Australia*; <sup>2</sup>*Australian Proteome Analysis Facility, Sydney, Australia*; <sup>3</sup>*Harvard Medical School, Boston, MA*
- PROTEOMICS: TISSUE**  
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- MP 503 **Differential Proteomics of *Pteropus* Wing Bones;** Timothy Cleland; Deepak Vashishth; *Rensselaer Polytechnic Inst, Troy, NY*
- MP 504 **Matching Therapies by Comparison of Kinase ATP Uptake in Lung Tumors and Drug Responses in Lung Cancer Cell Lines;** Bin Fang; Melissa Hoffman; Jiannong Li; Y. Ann Chen; Fumi Kinose; Katherine Fellows; Steven A. Eschrich; Uwe Rix; Eric B. Haura; John Koomen; *H. Lee Moffitt Cancer Center, Tampa, FL*
- MP 505 **Comparison of ATP Affinity Probe-based Kinome Enrichment at the Protein and Peptide Levels;** Yue Qi<sup>1</sup>; Abdullah Mallisho<sup>2</sup>; Danjun Ma<sup>1</sup>; Xiangmin Zhang<sup>1</sup>; Michael Caruso<sup>1</sup>; Divyasri Damacharla<sup>1</sup>; Nishit Shah<sup>1</sup>; Majed Abdullah Alharbi<sup>1</sup>; Berhane Seyoum<sup>2</sup>; Zhengping Yi<sup>1</sup>; <sup>1</sup>*Wayne State University, Detroit, MI*; <sup>2</sup>*University Health Center, Detroit, MI*
- MP 506 **Spatial and Temporal MSI and Proteomic Studies of Rat Spinal Cord Injury: Evidence of Caudal Segment for Possible Therapy Target;** Stéphanie Devaux<sup>1,2</sup>; Dasa Cizkova<sup>1,2</sup>; Maxence Wisztorski<sup>1</sup>; Lucia Slovinska<sup>2</sup>; Juraj Blasko<sup>2</sup>; Isabelle Fournier<sup>1</sup>; Michel Salzet<sup>1</sup>; <sup>1</sup>*INSERM U1192 - University of Lille 1, Villeneuve D'ascq Cedex, France*; <sup>2</sup>*Slovak Academy of Sciences, Kosice, Slovakia*
- MP 507 **Cell-type Specific Proteomics from Formalin-Fixed Paraffin Embedded (FFPE) Tissue: A Challenge?;** Shrutti Nayak; Eleanor Drummond; Thomas Wisniewski; Beatrix Ueberheide; *NYULMC, New York, NY*



- MP 508 **Proteomic and Bioinformatics Profile of Paired Human Alveolar Macrophages and Peripheral Blood Monocytes**; Kathleen C Lundberg; Sara Tomechko; Jessica Walrath; Mark Chance; Richard Silver; *Case Western Reserve University, Cleveland, OH*
- MP 509 **Developing and Assessing Polyacrylamide Hydrogel Technologies for Improved Protein Extraction from Targeted Regions of Biological Tissues**; David G. Rizzo<sup>1,3</sup>; Jessica L. Moore<sup>1,3</sup>; Boone M. Prentice<sup>2,3</sup>; Jeremy L. Norris<sup>2,3</sup>; Richard M. Caprioli<sup>1,3</sup>; <sup>1</sup>*Vanderbilt Dept. of Chemistry, Nashville, TN*; <sup>2</sup>*Vanderbilt Dept. of Biochemistry, Nashville, TN*; <sup>3</sup>*Vanderbilt University MSRC, Nashville, TN*
- MP 510 **Proteomic and Glycomic Analysis of the Mediodorsal Nucleus of Subjects with Schizophrenia**; Lilla Turiak<sup>1</sup>; Harry Pantazopoulos<sup>2,3</sup>; Nancy Leymarie<sup>1</sup>; Sabina Berretta<sup>2,3</sup>; Oliver D. King<sup>4</sup>; Joseph Zaia<sup>1</sup>; <sup>1</sup>*Boston University, Boston, MA*; <sup>2</sup>*Translational Neuroscience Laboratory, Mclean Hosp, Belmont, MA*; <sup>3</sup>*Department of Psychiatry, Harvard Medical School, Boston, MA*; <sup>4</sup>*Department of Cell and Developmental Biology UMass, Worcester, MA*
- MP 511 **Global Protein Profiling of Visceral Fat and Subcutaneous Fat from Obese Non-Diabetic and Obese T2D Subjects**; Danijun Ma; Alemu Fite; Xiangmin Zhang; Yue Qi; Michael Howard Wood; Rebecca Tagett; Sorin Draghici; Berhane Seyoum; Zhengping Yi; *Wayne State University, Detroit, MI*
- MP 512 **Evaluation of Sample Preparation Methods for Label-Free Quantitative Proteomics of Human Brain Tissue**; Kristin J. Boggio<sup>1</sup>; Marvin R. Natowicz<sup>2</sup>; John D. Leszyk<sup>1</sup>; Scott A. Shaffer<sup>1</sup>; <sup>1</sup>*University of Massachusetts Medical School, Worcester, MA*; <sup>2</sup>*Pathology & Laboratory Medicine, Cleveland Clinic, Cleveland, OH*
- MP 513 **Genotype-Tissue-Protein: Quantitative Proteomic Analysis of Human Tissue Proteome**; Lulu Cao; Michael Snyder; *Stanford University, Stanford, CA*
- MP 514 **MALDI Imaging-driven Microproteomics Workflow to Study Intra-Tumor Heterogeneity**; Deborah Alberts<sup>1</sup>; Charles Pottier<sup>2</sup>; Nicolas Smargiasso<sup>1</sup>; Gabriel Mazzucchelli<sup>1</sup>; Dominique Baiwir<sup>3</sup>; Philippe Delvenne<sup>2</sup>; Edwin De Pauw<sup>1</sup>; Rémi Longuespée<sup>1</sup>; <sup>1</sup>*Mass Spectrometry Laboratory, University Of Liège, Liège, Belgium*; <sup>2</sup>*Department of pathology, University of Liège, Liège, Belgium*; <sup>3</sup>*GIGA Proteomics Facility, University of Liège, Liège, Belgium*
- MP 515 **SWATH-MS Profiling of FFPE Tissue Sections**; Sean McMillan; Kristin Reinsvold; Jayme Wiederin; Melinda Wojtkiewicz; Weizhe Li; Howard E. Gendelman; Larisa Poluektova; Pawel Ciborowski; *University of Nebraska Medical Center, Omaha, NE*
- PROTEOMICS: QUANTITATIVE – LABEL FREE QUANTIFICATION 516 – 542**
- MP 516 **Quantitative Analysis of Membrane-Enriched and Soluble Proteome of Cortex from Mice Exposed to Psychotropic Medication**; Cátia Santa<sup>1,2</sup>; Susana C. Saraiva<sup>1,3</sup>; Sandra Anjo<sup>1,4</sup>; Vera M. Mendes<sup>1,5</sup>; Graça Baltazar<sup>6</sup>; Michael J. Dunn<sup>7</sup>; David Cotter<sup>8</sup>; Bruno Manadas<sup>1,5</sup>; <sup>1</sup>*Center for Neurosciences and Cell Biology, Coimbra, Portugal*; <sup>2</sup>*Institute for Interdisciplinary Research, Coimbra, Portugal*; <sup>3</sup>*Faculty of Pharmacy, University of Coimbra, Coimbra, Portugal*; <sup>4</sup>*Faculty of Sciences and Technology, Coimbra, Portugal*; <sup>5</sup>*Biocant - Biotechnology Innovation Center, Cantanhede, Portugal*; <sup>6</sup>*CICS-UBI - Health Sciences Research Center, Covilhã, Portugal*; <sup>7</sup>*Proteome Research Centre, University College, Dublin, Ireland*; <sup>8</sup>*Department Psychiatry, Royal College of Surgeons, Dublin, Ireland*
- MP 517 **Proteomic Analysis of Superior Frontal Gyrus from Brains of Humans with Mild Cognitive Impairment and Alzheimer's Disease**; Dale Chaput; Lisa Kirouac; Jaya Padmanabhan; Stanley M. Stevens, Jr; *University of South Florida, Tampa, Florida*
- MP 518 **How Many Proteins can be Measured and Quantified from 1000 and 5000 Cells?**; Beom-Jun Kim; Sung Yun Jung; Jong Min Choi; Jun Qin; *Baylor College of Medicine, Houston, Texas*
- MP 519 **Osteoblast-released Matrix Vesicle Activity and Composition are Regulated by Sulfated Glycosaminoglycans**; Johannes Schmidt<sup>1,2</sup>; Stefanie Kliemt<sup>1,3</sup>; Carolin Preissler<sup>4</sup>; Stephanie Möller<sup>5</sup>; Martin von Bergen<sup>1,6</sup>; Ute Hempel<sup>4</sup>; Stefan Kalkhof<sup>1</sup>; <sup>1</sup>*Helmholtz Centre for Environmental Research - UFZ, Leipzig, Germany*; <sup>2</sup>*Institute of Biochemistry, Leipzig University, Leipzig, Germany*; <sup>3</sup>*B CUBE Center for Molecular Bioengineering, Dresden, Germany*; <sup>4</sup>*Institute of Physiological Chemistry, TU Dresden, Dresden, Germany*; <sup>5</sup>*Biomaterials Department, INNOVENT e.V., Jena, Germany*; <sup>6</sup>*Department of Biotechnology, Aalborg University, Aalborg, Denmark*
- MP 520 **Label-free Quantitative Hippocampal Proteomics Reveals Pathways Linking Gamma Radiation Damage to Pathways Associated with Mitochondrial Function, Synaptic Activity and Memory**; Lin Huang<sup>1</sup>; Samantha Wickramasekara<sup>1</sup>; Jacob Rabe<sup>2</sup>; Claudia Maier<sup>1</sup>; <sup>1</sup>*Department of Chemistry, Oregon State University, Corvallis, OR*; <sup>2</sup>*Behav Neurosci, Neurol, Radiat Med, OHSU, Portland, OR*
- MP 521 **Proteomics Analysis of Altered Cellular Metabolism Induced by Insufficient Copper Level**; Sohye Kang; Gang Xiao; Da Ren; Zhongqi Zhang; Nicole Le; Michael Trentalange; Shivani Gupta; Henry Lin; Pavel Bondarenko; *Amgen, Inc., Thousand Oaks, CA*
- MP 522 **Identification of LRRK2 Substrates in a Drosophila Melanogaster Model of Parkinson's Disease**; William Edelman; Leo Pallanck; Judit Villen; *University of Washington, Seattle, WA*
- MP 523 **Protein Quantitation False Discovery Rates and Environmental Proteomics**; Paul A. Haynes; David Handler; Iniga Seraphina George; Samantha Emery; YunQi Wu; Vineet Vaibhav; Mehdi Mirzaei; *Macquarie University, North Ryde, Sydney, Australia*
- MP 524 **Proteomics-driven Exploration of Hypoxia-responsive Cellular Pathways associated to Metastasis in Osteosarcoma**; Zifeng Song<sup>1</sup>; Liping Yang<sup>1</sup>; Jeffrey Morre<sup>1</sup>; Milan Milovancev<sup>2</sup>; Siva Kolluri<sup>3</sup>; Claudia Maier<sup>1</sup>; <sup>1</sup>*Department of Chemistry, Oregon State University, Corvallis, Oregon*; <sup>2</sup>*College of Veterinary, Oregon State University, Corvallis, OR*; <sup>3</sup>*Department of Env.&Mol. Tox, Oregon State University, Corvallis, OR*
- MP 525 **Peptide Selection for Targeted Proteomics Quantitation: The Wisdom of the Crowds**; Cristina Chiva<sup>1,2</sup>; Eduard Sabidó<sup>1,2</sup>; <sup>1</sup>*Proteomics Unit (CRG), Barcelona, Spain*; <sup>2</sup>*University Pompeu Fabra (UPF), Barcelona, Spain*
- MP 526 **Protein Profiling (HDMS<sup>E</sup>) for Monitoring of Chondrocyte Differentiation of Mesenchymal Stem Cells in 3D Pellet Culture in a Multi-Omic Approach**; Shujuan Tao; Andrea R. Tan; David Chen; Clark T. Hung; Lewis M. Brown; *Columbia University, New York, NY*
- MP 527 **Use of High Resolution Accurate Mass (HRAM) MS1 to Test RNA – Interference Mediated Protein Suppression in Western Corn Rootworm**; David Mccaskill<sup>1</sup>; Tao Xu<sup>1</sup>; Sek Yee Tan<sup>1</sup>; Murugesan Rangasamy<sup>1</sup>; James Hasler<sup>1</sup>; Haichuan Wang<sup>2</sup>; Ana Maria Velez Arango<sup>2</sup>; Hong Chen<sup>2</sup>; Jessica Jurzenski<sup>2</sup>; Narva Kenneth<sup>1</sup>; Blair Siegfried<sup>2</sup>; <sup>1</sup>*Dow AgroSciences, Indianapolis, IN*; <sup>2</sup>*University of Nebraska, Lincoln, NE*
- MP 528 **Measuring Time-Dependent Effects of Ionizing Radiation on Mammalian Tissue Using Quantitative Proteomics**; Dyna I. Shirasaki; William McBride; Joseph Capri; Elizabeth Singer; Julian Whitelegge; Joseph A. Loo; *UCLA, Los Angeles, CA*



# MONDAY POSTERS

- MP 529 **Very Deep Coverage of the Human Proteome using a Very High Resolution Quadrupole Time-Of-Flight Instrument**; Scarlet Beck<sup>1</sup>; [Florian Meier](#)<sup>1</sup>; Annette Michalski<sup>2</sup>; Oliver R  ther<sup>2</sup>; Markus Lubeck<sup>2</sup>; Stephanie Kaspar<sup>2</sup>; Igor Paron<sup>1</sup>; J  rgen Cox<sup>1</sup>; Matthias Mann<sup>1</sup>; <sup>1</sup>Max-Planck-Institute of Biochemistry, Martinsried (near Munich), Germany; <sup>2</sup>Bruker Daltonik GmbH, Bremen, Germany
- MP 530 **Brain Organelle Proteomics: DDA and SWATH Based Quantifications of Biochemically Isolated Mouse Brain Synapse Sub-Fractions**; [Nikhil J. Pandya](#)<sup>1</sup>; Frank Koopmans<sup>2</sup>; August B. Smit<sup>1</sup>; Ka wan Li<sup>1</sup>; <sup>1</sup>Dept. of Molecular Cellular Neurobiology, CNCR, VU, Amsterdam, The Netherlands; <sup>2</sup>Dept. of Functional Genomics, CNCR, VU, Amsterdam, The Netherlands
- MP 531 **Knockdown and Overexpression of Phosphohistidine Phosphatase 1 Leads to Alterations in the Proteome of a Mouse Hepatocyte Cell Line**; [Ashley Culver-Cochran](#); Stanley M. Stevens, Jr; *University of South Florida, Tampa, FL*
- MP 532 **MS1-based Label-Free Proteomics using a Quadrupole Orbitrap Mass Spectrometer**; Tali Shalit; Dalia Elinger; Alon Savidor; Alexandra Gabashvili; [Yishai Levin](#); *Weizmann Institute of Science, Rehovot, Israel*
- MP 533 **Mapping the DNA Damage Response to the Temporal Occurrence of Histone Modifications**; Kevin Leahy; *Durham, NH*
- MP 534 **Comprehensive Relative Quantification of the Cytochromes P450 using SWATH™ Acquisition**; Rosalind E. Jenkins<sup>1</sup>; [Sibylle Heidelberger](#)<sup>2</sup>; Thomas Knapman<sup>2</sup>; Francesco L. Brancia<sup>2</sup>; Neil R Kitteringham<sup>1</sup>; B. Kevin Park<sup>1</sup>; <sup>1</sup>University of Liverpool, Liverpool, UK; <sup>2</sup>Sciex, Warrington, UK
- MP 535 **In-depth Proteomic Analysis of Sorafenib-induced Resistance in Human Hepatocellular Carcinoma with Subcellular Fractionation**; [Joon-Ho Park](#)<sup>1</sup>; Dohyun Han<sup>1,3</sup>; Su Jong Yu<sup>2</sup>; Jung-Hwan Yoon<sup>2</sup>; Youngsoo Kim<sup>1,4</sup>; <sup>1</sup>Department of Biomedical Engineering, SNUH, Seoul, Korea; <sup>2</sup>Department of Internal Medicine, SNUH, Seoul, Korea; <sup>3</sup>Biomedical Research Institute, SNUH, Seoul, Korea; <sup>4</sup>Institute of Medical & Bioengineering MRC, SNU, Seoul, Korea
- MP 536 **Absolute Protein Quantification of Starved *Bacillus subtilis* during Adaptation to Oxidative Stress**; [Sandra Maa  ](#); Sarah Wettst  dt; Florian Bonn; Michael Hecker; D  rte Becher; *Institute for Microbiology, Ernst Moritz Arndt University Greifswald, Greifswald, Germany*
- MP 537 **Annotation of the Domestic Pig Genome by Quantitative Proteomics**; [Harald Marx](#)<sup>1,2</sup>; Hannes Hahne<sup>1</sup>; Susanne Ulbrich<sup>3</sup>; Angelika Schnieke<sup>1</sup>; Oswald Rottmann<sup>1</sup>; Dmitriy Frishman<sup>1</sup>; Bernhard Kuster<sup>1</sup>; <sup>1</sup>TU Muenchen, Freising, Germany; <sup>2</sup>University of Wisconsin, Madison, WI; <sup>3</sup>ETH Zurich, Zurich, Switzerland
- MP 538 **Investigating the Effect of Estrogen on Renal Cell Carcinoma with Different VHL Genetic Backgrounds using Quantitative Proteomics**; [Wei-Chi Ku](#)<sup>1</sup>; Chi-Jung Huang<sup>1,2</sup>; Shao-Kuan Chen<sup>2</sup>; <sup>1</sup>Fu Jen Catholic University, New Taipei, Taiwan; <sup>2</sup>Cathay General Hospital, Taipei, Taiwan
- MP 539 **IFIX is a Viral DNA Sensor Acting in Defense against Human DNA Viruses**; [Marni Crow](#); Tuo Li; Benjamin Diner; Ileana M. Cristea; *Princeton University, Princeton, NJ*
- MP 540 **Drug-inducing Cell Death Mechanics is Rigid: A Proteomics Study**; [Alexey Chernobrovkin](#)<sup>1</sup>; Consuelo Vicente<sup>2</sup>; Neus Visa<sup>2</sup>; Roman Zubarev<sup>1</sup>; <sup>1</sup>Karolinska Institute, Stockholm, Sweden; <sup>2</sup>Stockholm University, Stockholm, Sweden
- MP 541 **A Hybrid Virology-Proteomics Approach Defines the Mechanisms of Cellular Immune Response to Viral DNA**; [Benjamin A. Diner](#); Tuo Li; Krystal K. Lum; Todd M. Greco; Marni S. Crow; Ileana M. Cristea; *Princeton University, Princeton, NJ*
- MP 542 **Global Proteomic Analysis of Ovarian High-Grade Serous Carcinomas using SWATH-MS for Targeted Verification of Proteome Changes Associated with Genomic Alterations**; [Stefani Thomas](#); Paul Aiyetan; Li Chen; Zhen Zhang; Daniel Chan; Hui Zhang; *Johns Hopkins University, Baltimore, MD*
- PROTEOMICS: CLINICAL APPLICATIONS  
543 - 569**
- MP 543 **Proteomics Identifies Distinct Immunoglobulin Light Chain Variable Region Usage in Clinical Subsets of Amyloidosis**; [Surendra Dasari](#)<sup>1</sup>; Jason D Theis<sup>1</sup>; Julie Vrana<sup>1</sup>; Ahmet Dogan<sup>2</sup>; Paul Kurtin<sup>1</sup>; <sup>1</sup>Mayo Clinic, Rochester, MN; <sup>2</sup>Memorial Sloan Kettering Cancer Center, New York, NY
- MP 544 **The Structure and Function of the Synaptic Proteome Vary by Sex, Neuropsychiatric Disease Diagnosis, and Brain Region**; [Stephanie L. Willard](#)<sup>1</sup>; Anamika Banerjee<sup>1</sup>; Ailin Cao<sup>1</sup>; Karin E. Borgmann-Winter<sup>1,2</sup>; Chang-Gyu Hahn<sup>1</sup>; <sup>1</sup>University of Pennsylvania Dept of Psychiatry, Philadelphia, PA; <sup>2</sup>Children's Hospital of Philadelphia, Philadelphia, PA
- MP 545 **Effect of Ion Mobility Measurements on the MS Analyses of Proteins Associated with Autoimmune Diseases**; Jeffrey F. Kuhn<sup>1</sup>; [Leesa Deterding](#)<sup>2</sup>; <sup>1</sup>NIEHS/NIH/DHHS, Research Triangle Park, NC; <sup>2</sup>NIEHS, RTP, NC
- MP 546 **Quantitative Measurements of a Specific Hydroxylated Collagen Peptide in Urine Improves the Detection of Colorectal Liver Metastases**; [Nick Van Huizen](#); Zarina Lalmahomed; Mirelle Broker; Robert Coebergh van den Braak; Jan IJzermans; Theo Luider; Lennard Dekker; *Erasmus Medical Center, Rotterdam, the Netherlands*
- MP 547 **Investigating the Contribution of Karyotype Changes to Multidrug Resistance using Quantitative Proteomics**; [Lilian Kabeche](#)<sup>1,2</sup>; Andrew Grasseti<sup>1,2</sup>; Mark Adamo<sup>1</sup>; Scott Gerber<sup>1,2</sup>; <sup>1</sup>Norris Cotton Cancer Center, Lebanon, New Hampshire; <sup>2</sup>Geisel School of Medicine at Dartmouth, Hanover, NH
- MP 548 **The Function of Pathogenic Human Torsin A**; [Jong Bok Seo](#); Soo Jeong Park; *Korea Basic Science Institute, Seoul, South Korea*
- MP 549 **Accurate Clinical Detection of Hemoglobin Variants via Combined Top-Down and Bottom-Up Proteomics**; [Raymond Moore](#); Roman Zenka; Patricia Wendt; Kenneth Swanson; Jennifer Oliveira; James Hoyer; Surendra Dasari; *Mayo Clinic, Rochester, MN*
- MP 550 **Selective Proteomics Analysis Using Congo Red as a Precipitating Reagent**; [Hongwu Jing](#)<sup>1</sup>; Irina A. Buhimschi<sup>2,3</sup>; Guomao Zhao<sup>2</sup>; Michelle Axe<sup>4</sup>; Catalin S. Buhimschi<sup>3</sup>; Vicki Wysocki<sup>1</sup>; <sup>1</sup>Dept. Chem. Biochem., The Ohio State University, Columbus, OH; <sup>2</sup>Research Inst. at Nationwide Children's Hospital, Columbus, OH; <sup>3</sup>Dept. OB/GYN, The Ohio State University, Columbus, OH; <sup>4</sup>Dept. Biochem. Mol. Biol., Otterbein University, Westerville, OH
- MP 551 **Determination of EGFR and VEGF Signaling Pathway Activity by immuno-MALDI to Predict the Outcome of Targeted Colorectal Cancer (CRC) Treatment**; [Robert Popp](#)<sup>1</sup>; Andrew Chambers<sup>1</sup>; Adriana Aguilar-Mahecha<sup>2</sup>; Oliver P  tz<sup>3</sup>; Mark Basik<sup>2</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>UVic - Genome BC Proteomics Centre, Victoria, Canada; <sup>2</sup>Jewish General Hospital, McGill University, Montreal, Canada; <sup>3</sup>Natural and Medical Sciences Institute (NMI), Reutlingen, Germany
- MP 552 **Absolute Quantification of Proteins from Different Types of Dried Blood Spot (DBS) Cards using LC-MS/MS**; [Jerome Vialaret](#)<sup>1</sup>; Christophe Hirtz<sup>1</sup>; Karine Hirtz<sup>3</sup>; Alan Barnes<sup>4</sup>; Audrey Gabelle<sup>2</sup>; Sylvain Lehmann<sup>1</sup>; <sup>1</sup>LBPC-IRB, CHU de Montpellier, Montpellier, France; <sup>2</sup>Centre M  moire Ressources Recherche, Montpellier, France; <sup>3</sup>Spot to Lab, Cap Om  ga, Montpellier, France; <sup>4</sup>Shimadzu Research Laboratory, Manchester, UK



- MP 553 **From Venome to Syndrome: Using Mass Spectrometry to Understand the Correspondence of Rattlesnake Venom Composition and Clinical Symptoms of Snakebite**; William K. Hayes<sup>1</sup>; Aaron Corbit<sup>1</sup>; Sean P. Bush<sup>3</sup>; Eric C.K. Gren<sup>1</sup>; Allen M. Cooper<sup>1</sup>; Chip Cochran<sup>1</sup>; Gerard A. Fox<sup>1</sup>; Carl E. Person<sup>1</sup>; Wayne Kelln<sup>1</sup>; Kevin Kim<sup>2</sup>; Zachary Travis<sup>2</sup>; Ben D. Gardner<sup>1</sup>; <sup>1</sup>Loma Linda University, Loma Linda, CA; <sup>2</sup>La Sierra University, Riverside, CA; <sup>3</sup>East Carolina University, Greenville, NC
- MP 554 **Quantitative Proteomic Discovery of Candidate Serum Biomarkers for Early Detection of Ovarian Cancer**; Matthew Russell<sup>1,4</sup>; Michael Walker<sup>1,4</sup>; Andrew Williamson<sup>1</sup>; Aleksandra Gentry-Maharaj<sup>2</sup>; Andy Ryan<sup>2</sup>; Evangelia-Ourlana Fourkala<sup>2</sup>; Phillip Humphryes<sup>1</sup>; Usha Menon<sup>2</sup>; Anthony Whetton<sup>1</sup>; Ian Jacobs<sup>1,3</sup>; Robert Graham<sup>1</sup>; <sup>1</sup>University of Manchester, Manchester, UK; <sup>2</sup>University College London, London, UK; <sup>3</sup>University of New South Wales, Sydney, Australia
- MP 555 **Bottom-up Proteomic Analysis of Single HCT 116 Colon Carcinoma Multicellular Spheroids**; Peter Feist<sup>1,2</sup>; Xin Liu<sup>1</sup>; Liangliang Sun<sup>1</sup>; Norman Dovichi<sup>1</sup>; Amanda Hummon<sup>1,2</sup>; <sup>1</sup>University of Notre Dame, Notre Dame, Indiana; <sup>2</sup>Integrated Biomedical Sciences Program, Notre Dame, IN
- MP 556 **Zoledronic Acid Potentiates  $\gamma\delta$  T-Cell Anti-Leukemic Activity in Patients Receiving  $\alpha\beta$  T and CD19+ Depleted Grafts from Haplo-Identical Donors**; Andrea Petretto<sup>1</sup>; Irma Airoidi<sup>1</sup>; Chiara Lavarello<sup>1</sup>; Elvira Inglesel<sup>1</sup>; Alice Bertaina<sup>2</sup>; Barbarella Lucarelli<sup>2</sup>; Alessia Zorzoli<sup>1</sup>; Pietro Merli<sup>2</sup>; Giulia Barbarito<sup>2</sup>; Letizia Brescia<sup>2</sup>; Valentina Bertaina<sup>2</sup>; Giuseppe Milano<sup>2</sup>; Franco Locatelli<sup>2</sup>; <sup>1</sup>Institute Giannina Gaslini, Genoa, Italy; <sup>2</sup>Bambino Gesù Children's Hospital, Rome, Italy
- MP 557 **Barcoding Primary Human B-cells via Analysis of Membrane Proteins on the Cell Surface**; Nicole A. Haverland<sup>1</sup>; Matthew Waas<sup>2</sup>; Tim Toby<sup>1</sup>; Ioanna Ntai<sup>1</sup>; Rebekah Gundry<sup>2</sup>; Neil L. Kelleher<sup>1</sup>; <sup>1</sup>Northwestern University, Evanston, IL; <sup>2</sup>Medical College of Wisconsin, Milwaukee, WI
- MP 558 **Detecting Recombinant Insulin Drugs in Amyloid Plaques of Diabetes Patients using Shotgun Proteomics**; Jason D Theis; Surendra Dasari; Julie Vrana; Roman Zenka; Paul Kurtin; *Mayo Clinic, Rochester, MN*
- MP 559 **Nanomaterial Based Sub-Proteome Selection for Analysis of the Activation State Of Macrophages**; Arnaud Millet; Magali Court; Adrien Mombrun; Vera Aiello; Frederic-Xavier Gaillard; Francois Berger; Ali Bouamrani; *Grenoble, France*
- MP 560 **The Associations between Enterovirus Infections and Type 1 Diabetes**; Niina Lietzen<sup>1</sup>; Sami Oikarinen<sup>2</sup>; Young Ah Goo<sup>3</sup>; David Goodlett<sup>3</sup>; Jorma Toppari<sup>1</sup>; Jorma Ilonen<sup>1</sup>; Riitta Veijola<sup>4</sup>; Mikael Knip<sup>5,6</sup>; Heikki Hyöty<sup>2</sup>; Riitta Lahesmaa<sup>1</sup>; <sup>1</sup>University of Turku, Turku, Finland; <sup>2</sup>University of Tampere, Tampere, Finland; <sup>3</sup>University of Maryland, Baltimore, Maryland; <sup>4</sup>University of Oulu, Oulu, Finland; <sup>5</sup>Children's Hospital, University of Helsinki, Helsinki, Finland; <sup>6</sup>Helsinki University Central Hospital, Helsinki, Finland
- MP 561 **Measuring Minimum Residual Disease in Multiple Myeloma by LC-MS/MS; A comparison to Multicolor Flow Cytometry**; H. Robert Bergen, III<sup>1</sup>; Angela Dispenzieri<sup>1</sup>; John Mills<sup>2</sup>; David Barnidge<sup>2</sup>; David Murray<sup>2</sup>; <sup>1</sup>Mayo Clinic, Rochester, MN; <sup>2</sup>Mayo Clinic / DLMP, Rochester, MN
- MP 562 **Diagnostic Accuracy for Proteomic Cancer Markers in the Face of Autoantibodies: Can We Assume Trypsin Does All the Work?** Christopher Shuford; Patricia Holland; Russell Grant; *Laboratory Corporation of America, Burlington, NC*
- MP 563 **Mass Spectrometry-based Phosphoproteomics for the Identification of Phosphorylation Signaling Pathways in Chronic Lymphocytic Leukemia (CLL)**; Stephen Swatkoski; Sarah Herman; Deanna Wong; Adrian Wiestner; Marjan Gucek; *-NIH/NHLBI, Bethesda, MD*
- MP 564 **Tandem MS/MS with Isotope Dilution Identifies a Cluster of Proteins Implicated in Kidney Disease in HDL of Hemodialysis Subjects**; Baohai Shao; Ian de Boer; Philip S. Mayer; Leila Zelnick; Maryam Afkarian; Jay W. Heinecke; Jonathan Himmelfarb; *University of Washington, Seattle, WA*
- MP 565 **Ultrasensitive Tissue Proteomics using an Enhanced Workflow with Para-Magnetic Beads for Clinical Proteomics Research Applications**; Christopher Hughes; Melissa McConechy; David Huntsman; Gregg Morin; *British Columbia Cancer Agency, Vancouver, BC*
- MP 566 **Mass Spectrometry Based Study of Human Body Adaptation during the Space-flight and MARS 105 Days Isolation Experiment**; Irina Larina<sup>1</sup>; Alexey Kononikhin<sup>2,5</sup>; Lyudmila Pastushkova<sup>1</sup>; Igor Popov<sup>4,5</sup>; Alexander Bzhozovsky<sup>1</sup>; Igor Dobrokhotov<sup>1</sup>; Evgeny Tiys<sup>3</sup>; Vladimir Ivanisenko<sup>3</sup>; Eugene Nikolaev<sup>2,6</sup>; <sup>1</sup>Institute of Biomedical Problems RAS, Moscow, Russia; <sup>2</sup>Institute for Energy Problems of Chemical Physics, Moscow, Russia; <sup>3</sup>Institute of Cytology and Genetics SB RAS, Novosibirsk, Russia; <sup>4</sup>Emanuel Institute of Biochemical Physics, Moscow, Russia; <sup>5</sup>Moscow Institute of Physics and Technology, Moscow, Russia; <sup>6</sup>Skolkovo Institute of Science and Technology, Skolkovo, Russia
- MP 567 **Differential Proteomic Analysis of Human Saliva using Tandem Mass Tags for Gastric Cancer Detection**; Hua Xiao<sup>1</sup>; David T.W. Wong<sup>2</sup>; <sup>1</sup>Shanghai Jiao Tong University, Shanghai, China; <sup>2</sup>UCLA, CA
- MP 568 **Single Point Calibrator for Protein Quantification in Formalin-Fixed Paraffin Embedded Tissues**; Han-Yin Yang<sup>1</sup>; James G. Bollinger<sup>1</sup>; Ying Sonia Ting<sup>1</sup>; Christine Wu<sup>2</sup>; Andrew Hoofnagle<sup>1</sup>; Michael J. Maccoss<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Stratus Biosciences, Seattle, WA
- MP 569 **Developing a Robust Urine UMOD and Albumin Assay By Liquid Chromatography-Targeted Mass Spectrometry**; Qin Fu<sup>1</sup>; Eric Grote<sup>2</sup>; Jie Zhu<sup>2</sup>; Christine Jelinek<sup>3</sup>; Josef Coresh<sup>4</sup>; Jennifer Van Eyk<sup>1</sup>; <sup>1</sup>Cedars Sinai Medical Center, Los Angeles, CA; <sup>2</sup>Johns Hopkins University, Baltimore, MD; <sup>3</sup>Johns Hopkins School of Medicine, Baltimore, MD; <sup>4</sup>Johns Hopkins Bloomberg School of Public Health, Baltimore, MD
- PHOSHOPEPTIDES: ENRICHMENT METHODS**  
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- MP 570 **Quantitative Phosphoproteomics on a  $\mu$ g-scale - A Straightforward and Highly Sensitive ERLIC-SCX/RP-LC-MS Strategy**; Stefan Loroch<sup>1</sup>; Oliver Page<sup>1</sup>; René Zahedi<sup>1</sup>; Albert Sickmann<sup>1,2</sup>; <sup>1</sup>Leibniz-Institut für Analytische Wissenschaften, Dortmund, Germany; <sup>2</sup>University of Aberdeen, Aberdeen, Scotland
- MP 571 **Automation Enables Highly Reproducible Phosphopeptide Enrichment from Complex Mixtures by IMAC using High-Capacity Fe(III)-NTA Microchromatography Cartridges**; Jason Russell; Steve Murphy; *Agilent Technologies, Inc., Madison, WI*
- MP 572 **Spatial Extraction and Enrichment of Phosphopeptides from Tissues using Hydrogels Containing Metal Ion-functionalized Nanopolymers**; M. Lisa Manier; Jamie Wenke; Jeremy L. Norris; Kevin L. Schey; Richard Caprioli; *Vanderbilt University, Nashville, TN*
- MP 573 **Single Shot Phosphoproteomics**; Alex Hebert; Nicholas Kwiecien; Alicia Richards; Anna Merrill; Michael S. Westphall; Joshua J. Coon; *University of Wisconsin-Madison, Madison, WI*

- MP 574 **Enrichment of Phosphorylated Peptides using Polymeric Reverse Micelles for MALDI-MS Analysis;** Meizhe Wang; Bo Zhao; Mijanur Rahaman; Sankaran Thayumanavan; Richard Vachet; *University of Massachusetts Amherst, Amherst, MA*
- MP 575 **In-Depth Phosphoproteome Analysis in *E.coli* Using High-pH Reversed-Phase and TiO<sub>2</sub> Chromatography;** Gerhard Saalbach<sup>1</sup>; Sivaramesh Wigneshweraraj<sup>2</sup>; Rita Figueira<sup>2</sup>; <sup>1</sup>*John Innes Centre, Norwich, UK*; <sup>2</sup>*Imperial College, London, UK*
- MP 576 **PTM- and Protein-Based Proteome Profiling of Drug Response in Human Gastric Carcinoma Cells using Antibody-Based and Metal Affinity-Based Phosphopeptide Enrichment;** Matthew P. Stokes<sup>1</sup>; Charles L. Farnsworth<sup>1</sup>; Hongbo Gu<sup>1</sup>; Jian Min Ren<sup>1</sup>; Vicky Yang<sup>1</sup>; Camilla R. Worsfold<sup>2</sup>; Kimberly A. Lee<sup>1</sup>; Jeffrey C. Silva<sup>1</sup>; <sup>1</sup>*Cell Signaling Technology, Danvers, MA*; <sup>2</sup>*Emory University, Atlanta, GA*
- MP 577 **Investigation of Changes in Protein Phosphorylation During Cell Differentiation: Combined Extraction-Fractionation at High pH to Facilitate Phosphopeptide Isolation;** Alice Harnacke<sup>1,2</sup>; Wolfgang Fischer<sup>1</sup>; <sup>1</sup>*The Salk Institute, La Jolla, CA*; <sup>2</sup>*University of Freiburg, Freiburg, Germany*
- MP 578 **StageTip-based IMAC for Rapid and Deep Phosphoproteomic Typing in One-Shot LC-MS/MS Analysis;** Chia-Feng Tsai; Yi-Ting Wang; Miao-Hsia Lin; Pei-Yi Lin; Yu-Ju Chen; *Academia Sinica, Taipei, Taiwan*
- MP 579 **Comparing Multi-Step IMAC and Multi-Step TiO<sub>2</sub> Methods for Phosphopeptide Enrichment;** Xiaoshan Yue; Amanda B. Hummon; *University of Notre Dame, Notre Dame, IN*
- MP 580 **Tyrosine Phosphorylation Profiling and Phosphoproteome Mapping of Three Mouse Tissues;** Ling Zhong; Mark Raftery; *UNSW, Sydney, Australia*
- GLYCOPROTEINS: METHOD DEVELOPMENT**  
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- MP 581 **Automated Structural Characterization of Intact N- and O-linked Glycopeptide using a Orbitrap Fusion Tribrid Mass Spectrometer;** Chein-Hung Chen; Ya-Ping Lin; Fang-Chi Liu; Chi-Lin Wu; Jung-Lee Lin; Chung-Hsuan Chen; *Academia Sinica, Taipei, Taiwan*
- MP 582 **Glycan Composition and Charge State Influence upon Collision Cross Sections of High Mannose N-Linked Glycopeptides;** Abby S. Gelb; Eric D. Dodds; *University of Nebraska - Lincoln, Lincoln, NE*
- MP 583 **Glycoproteomic and Proteomic Analyses of Hearts from Hypertrophic Cardiomyopathy Mice;** Shuang Yang<sup>1</sup>; Sumita Mishra<sup>2</sup>; Lijun Chen<sup>1</sup>; Jian-Ying Zhou<sup>1</sup>; Yuri Poluektov<sup>1</sup>; Daniel W. Chan<sup>1</sup>; Subroto Chatterjee<sup>2</sup>; Hui Zhang<sup>1</sup>; <sup>1</sup>*John Hopkins Dept. of Pathology, Baltimore, MD*; <sup>2</sup>*Department of Pediatrics, Johns Hopkins University, Baltimore, MD*
- MP 584 **Effects of Charge Carrier and Composition on the Energy-Resolved Collision-Induced Dissociation of Tryptic N-Glycopeptides;** Forouzan Aboufazeli; Venkata Kolli; Abby S. Gelb; Eric D. Dodds; *University of Nebraska - Lincoln, Lincoln, NE*
- MP 585 **Improving the ETD Performance of Glycopeptides through Chemical Charge Enhancement;** William Alley; Yanyan Qu; Rebecca Sosa; *University of Texas at San Antonio, San Antonio, TX*
- MP 586 **High-Throughput Profiling of Protein N-Glycosylation by MALDI-TOF-MS Employing Linkage-Specific Sialic Acid Esterification;** Karli Reiding<sup>1</sup>; Dennis Blank<sup>1</sup>; Dennis Kuijper<sup>2</sup>; André Deelder<sup>1</sup>; Manfred Wuhrer<sup>1,2</sup>; <sup>1</sup>*Leiden University Medical Center, Leiden, Netherlands*; <sup>2</sup>*VU University, Amsterdam, Netherlands*
- MP 587 **Analysis of Site-specific N/O-Glycosylation of Targeted Proteins;** Shu-Hui Chen; *National Cheng Kung University, Tainan, Taiwan*
- MP 588 **O-linked Glycopeptide Analysis via Negative Electron Transfer Dissociation;** Nicholas M. Riley<sup>1</sup>; Nichollas E. Scott<sup>2</sup>; Mario F. Feldman<sup>3</sup>; Michael S. Westphall<sup>1</sup>; Joshua J. Coon<sup>1</sup>; <sup>1</sup>*University of Wisconsin, Madison, Wisconsin*; <sup>2</sup>*Center for High-Throughput for Biology, UBC, Vancouver, Canada*; <sup>3</sup>*Alberta Glycomics Centre, Dept. of Biology, Edmonton, Canada*
- MP 589 **Characterization of Intact Prostate Specific Antigen (PSA) and Its Glycoforms by CESI-MS under Native and Denaturing Conditions;** Marcia R. Santos<sup>1</sup>; Chitra K. Ratnayake<sup>1</sup>; David M. Horn<sup>2</sup>; Barry L. Karger<sup>3</sup>; Alexander R. Ivanov<sup>3</sup>; Rosa I. Viner<sup>2</sup>; <sup>1</sup>*Sciex, Brea, CA*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>3</sup>*Northeastern University, Boston, MA*
- MP 590 **N-glycan Analysis: Combining the Power of a Novel Glycan Label and Customized Scientific Library for Confident Glycan Assignment;** Mark Hilliard<sup>1</sup>; Naoibh McLoughlin<sup>1</sup>; Pauline Rudd<sup>1</sup>; Ying Qing Yu<sup>2</sup>; <sup>1</sup>*NIBRT, Dublin, Ireland*; <sup>2</sup>*Waters Waters Corporation., Milford, MA*
- MP 591 **Highly Specific Enrichment of N-glycoproteome through Nonreductive Amination Reaction using Fe<sub>3</sub>O<sub>4</sub>@SiO<sub>2</sub>-Aniline Nanoparticles;** Ying Zhang; Liqi Xie; Haojie Lu; *Fudan University, Shanghai, China*
- MP 592 **Glycosylation Patterns on HIV-1 Envelope Glycoprotein and Its Structural Implications;** Audra Laube<sup>1</sup>; Milan Raska<sup>1,2</sup>; Qing Wei<sup>1</sup>; Barbora Knoppova<sup>2</sup>; Stacy Hall<sup>1</sup>; Katerina Zachova<sup>2</sup>; Zhi-Qiang Huang<sup>1</sup>; Zina Moldoveanu<sup>1</sup>; Jan Novak<sup>1</sup>; Matthew Renfrow<sup>1</sup>; <sup>1</sup>*University of Alabama at Birmingham, Birmingham, AL*; <sup>2</sup>*Palacky University in Olomouc, Olomouc, Czech Republic*
- MP 593 **In-planta Deglycosylation and Mass Spectrometry;** Ranjith Muniguntti; Lindsay Bennett; Brian Berquist; Vally Kommineni; Earl White; Sylvain Marcel; *Caliber Biotherapeutics, Bryan, TX*
- MP 594 **Site-specific N- and O-glycosylation Analysis of Human IgG3 Assisted by Integrated C18-PGC-LC-ESI-MS/MS Analysis;** Kathrin Stavenhagen<sup>1</sup>; Rosina Plomp<sup>2</sup>; Gillian Dekkers<sup>3</sup>; Yoann Rombouts<sup>2,4</sup>; Paul J. Hensbergen<sup>2</sup>; Gestur Vidarsson<sup>3</sup>; Manfred Wuhrer<sup>1,2</sup>; <sup>1</sup>*BioAnalytical Chemistry, VU University Amsterdam, Amsterdam, The Netherlands*; <sup>2</sup>*CPM, Leiden University Medical Center, Leiden, The Netherlands*; <sup>3</sup>*Sanquin Research and Academic Medical Center, Amsterdam, The Netherlands*; <sup>4</sup>*Dep. Rheumatology, Leiden University Medical Center, Leiden, The Netherlands*
- MP 595 **An Improved Workflow using Rapid PNGase F to Quickly Deglycosylate IgG for Accurate N-glycan Analysis;** Paula Magnelli; Beth McLeod; Colleen McClung; Renpeng Liu; Alicia Bielik; Ellen Guthrie; *New England Biolabs, Ipswich, MA*
- MP 596 **High-Throughput Electron Capture Dissociation Mass Spectrometry in A Novel Branched Radio-Frequency Ion-Trap as a Platform for Glycoproteomics;** St John Skilton; J.C. Yves Leblanc; Takashi Baba; James Hager; J. Larry Campbell; *SCIEX, Concord, On, Canada*
- MP 597 **Development of a Novel Work Flow for the Enrichment of Glycated Peptides from Complex Matrices;** Sara Eun Lendal; Johannes Graumann; *Weill Cornell Medical College in Qatar, Doha, Qatar*
- MP 598 **Glycosylation of Vascular Endothelial Growth Factor Receptor 2 (VEGFR-2) in Angiogenesis;** Kevin Brown Chandler; Nader Rahimi; Catherine E Costello; *Boston University School of Medicine, Boston, MA*
- MP 599 **Site-specific Quantification of the Surface N-Sialoglycoproteome in Cancer Cells with Distinctive Invasiveness;** Weixuan Chen; Johanna Smeeckens; Ronghu Wu; *Georgia Tech, Atlanta, GA*





- MP 600 **Rapid Preparation of Released N-Glycans for HILIC Analysis Using a Novel Fluorescence and MS-Active Labeling Reagent;** Matthew Lauber<sup>1</sup>; Ying-Qing Yu<sup>1</sup>; Darryl Brousmiche<sup>1</sup>; Jeffrey Thomson<sup>2</sup>; Seamus O'Connor<sup>2</sup>; Zhengmao Hua<sup>1</sup>; Stephan Koza<sup>1</sup>; Paula Magnelli<sup>3</sup>; Ellen Guthrie<sup>3</sup>; Chris Taron<sup>3</sup>; Kenneth Fountain<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Regeneron Pharmaceuticals, Rensselaer, NY; <sup>3</sup>New England Biolabs, Ipswich, MA
- MP 601 **Site-Specific N-glycoform Analysis of Human Alpha1-Acid Glycoprotein: Towards an Integrated Approach for Complete Molecular Characterization;** Katherine N. Schumacher; Eric D. Dodds; *University of Nebraska - Lincoln, Lincoln, NE*
- MP 602 **A Novel Quantitative Mass Spectrometry Platform for Determining Site-Specific Protein O-GlcNAcylation Dynamics;** Xiaoshi Wang<sup>1</sup>; Zuo-Fei Yuan<sup>1</sup>; Jing Fan<sup>2</sup>; John M. Denu<sup>2</sup>; Benjamin A. Garcia<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA; <sup>2</sup>University of Wisconsin-Madison, Madison, WI
- MP 603 **A Systematic Investigation of CID Q-TOF-MS/MS Collision Energies to Improve N- and O-glycopeptide Identification by LC-MS/MS;** Hannes Hinneburg<sup>1,2</sup>; Kathrin Stavenhagen<sup>3</sup>; Ulrike Schweiger-Hufnagel<sup>4</sup>; Dirk Wunderlich<sup>4</sup>; Stuart Pengelley<sup>4</sup>; Arndt Asperger<sup>4</sup>; Wolfgang Jabs<sup>4</sup>; Peter H. Seeberger<sup>1,2</sup>; Daniel Varón Silva<sup>1</sup>; Manfred Wuhre<sup>3</sup>; Daniel Kolarich<sup>1</sup>; <sup>1</sup>Max-Planck-Institute of Colloids and Interfaces, Potsdam, Germany; <sup>2</sup>Free University Berlin, Berlin, Germany; <sup>3</sup>VU University Amsterdam, Amsterdam, Netherlands; <sup>4</sup>Bruker, Bremen, Germany
- MP 604 **Glycoproteomics by HILIC-FLR-MS<sup>n</sup> of Procainamide-Labeled Glycans;** Brian C. Gau; Benjamin Cutak; Kevin Ray; *Sigma-Aldrich, St. Louis, MO*
- MP 605 **Parallel Data Acquisition of In-source Fragmented Glycopeptides to Characterize the Peptide Backbones and Glycan Structures;** Jingfu Zhao; Ehwang Song; Yehia Mechref; *Texas Tech University, Lubbock, Texas*
- SYSTEMS BIOLOGY: PROTEOMICS**  
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- MP 606 **Comprehensive Characterization of the Differentiation of Human Embryonic Stem Cells into Mesenchymal Stem Cells;** Anja M Billing; Shaima S Dib; Hisham Ben-Hamidane; Aditya M Bhagwat; Shahina Hayat; Pankaj Kumar; Rasha Al-Mismar; Neha Goswami; Karsten Suhre; Arash Rafii; Johannes Graumann; *Weill Cornell Medical College in Qatar, Doha, Qatar*
- MP 607 **Subcellular Trafficking of Cholera Toxin Revealed by Proteome-wide Dose Response Time Course Profiling;** Christopher Ebmeier; Tristan McClure-Begley; Douglas Chapnick; Xuedong Liu; William Old; *University of Colorado, Boulder, CO*
- MP 608 **Regulation of the Primary Human Trophoblast Cell Secretome by Mechanistic Target of Rapamycin (mTOR) Signaling;** Susan T. Weintraub<sup>1</sup>; Frederick Rosario<sup>2</sup>; Sammy Pardo<sup>1</sup>; Thomas Jansson<sup>2</sup>; <sup>1</sup>Univ. of Texas Health Science Center, San Antonio, TX; <sup>2</sup>Univ. of Colorado Denver Anschutz Med. Campus, Aurora, CO
- MP 609 **The Nuclear Proteome of a Vertebrate;** Martin Wüthrich; Thomas Güttler; Leonid Peshkin; Graeme Mcalister; Matthew Sonnett; Aaron C. Groen; Marc Presler; Brian Erickson; Timothy J. Mitchison; Marc W. Kirschner; Steven Gygi; *Harvard Medical School, Boston, MA*
- MP 610 **Chemical and Computational Approaches to Integrate Redox Signaling in the Study of Systems Biology;** Nelmi O. Devarie-Baez; Zhiwei Ji; Elsa Silva-Lopez; Jade Mims; Xiaofei Chen; Allen W. Tsang; Xiaobo Zhou; Cristina M. Furdui; *Wake Forest School of Medicine, Winston-Salem, NC*
- MP 611 **The Dynamic Phosphoproteome of Peripheral Nerve Injury and Chronic Pain;** Christopher B. Lietz<sup>1</sup>; Dana M. Tilley<sup>2</sup>; Courtney Kelley<sup>2</sup>; Ricardo Vallejo<sup>2</sup>; Ramsin Benjamin<sup>2</sup>; Joseph Williams<sup>3</sup>; David L. Cedeño<sup>2,3</sup>; Lingjun Li<sup>1</sup>; <sup>1</sup>University of Wisconsin, Madison, WI; <sup>2</sup>Millennium Pain Center, Bloomington, IL; <sup>3</sup>Illinois Wesleyan University, Bloomington, IL
- MP 612 **Phosphoproteomic Analysis of Signal Integration in Cancer;** Robert Lawrence; Judit Villén; *University of Washington, Seattle, WA*
- MP 613 **Targeted Proteomics-Driven Computational Modeling of Macrophage S1P Chemosensing;** Nathan Manes<sup>1</sup>; Bastian Angermann<sup>1</sup>; Eunkyung An<sup>1</sup>; Virginie Sjoelund<sup>1</sup>; Jing Sun<sup>1</sup>; Masaru Ishii<sup>2</sup>; Ronald Germain<sup>1</sup>; Martin Meier-Schellersheim<sup>1</sup>; Aleksandra Nita-Lazar<sup>1</sup>; <sup>1</sup>NIH, Bethesda, MD; <sup>2</sup>Osaka University, Osaka, Japan
- MP 614 **Proteomic and Phosphoproteomic Characterization of Breast Cancer Progression in MCF10A Model Cell-line;** Hongjie Pan; Harsha P. Gunawardena; Xian Chen; *University of North Carolina at Chapel Hill, Chapel Hill, NC*
- MP 615 **Kinase Profiling, Expression Proteomics, and Phosphoproteomics Reveal Adaptive Signaling in Melanoma after Targeted Therapy;** Ritin Sharma<sup>1</sup>; Inna Fedorenko<sup>1</sup>; Bin Fang<sup>1</sup>; David Britton<sup>2</sup>; Sasa Koncarevic<sup>2</sup>; Gitte Boehm<sup>2</sup>; Ian Pike<sup>2</sup>; Keiran Smalley<sup>1</sup>; John Koomen<sup>1</sup>; <sup>1</sup>H. Lee Moffitt Cancer Center & Research Institute, Tampa, FL; <sup>2</sup>Proteome Sciences PLC, Surrey, UK
- MP 616 **Deep Proteomic and Phosphoproteomic Profiling Reveals Different Gliomagenesis Mechanism between Two Pediatric High-grade Glioma Subtypes;** Hong Wang<sup>1,2</sup>; Tim Shaw<sup>1</sup>; Xusheng Wang<sup>1</sup>; Yuxin Li<sup>1</sup>; Ji-Hoon cho<sup>1</sup>; Barbara Paugh<sup>1</sup>; Alex Diaz<sup>1,2</sup>; Yanling Yang<sup>1</sup>; Zhiping Wu<sup>1</sup>; Haiyan Tan<sup>1</sup>; Bing Bai<sup>1</sup>; Anthony High<sup>1</sup>; Vishwajeeth Pagala<sup>1</sup>; Suzanne Baker<sup>1,2</sup>; Junmin Peng<sup>1,2</sup>; <sup>1</sup>St Jude Children's Research Hospital, Memphis, TN; <sup>2</sup>University of Tennessee Health Science Center, Memphis, TN
- MP 617 **Global and Targeted Quantification of Seven Human Cell Lines Reveals the Correlation of Cell Type-Specific Responses with Feedback Regulators ;** Tujin Shi<sup>1</sup>; Yuqian Gao<sup>1</sup>; Matthew Gaffrey<sup>1</sup>; William Chrisler<sup>1</sup>; Thomas Fillmore<sup>1</sup>; Carrie Nicora<sup>1</sup>; Meng Markillie<sup>1</sup>; karin rodland<sup>1</sup>; Jason McDermott<sup>1</sup>; Mario Niepel<sup>2</sup>; Peter Sorger<sup>2</sup>; Richard Smith<sup>1</sup>; Steven Wiley<sup>1</sup>; Wei-Jun Qian<sup>1</sup>; <sup>1</sup>Pacific Northwest National Lab, Richland, WA; <sup>2</sup>Harvard Medical School, Boston, MA
- MP 618 **Metaproteomics Based on SWATH-MS Approach to Analyse a Complex Synthetic Microbial Community;** Mélanie Béraud; giuseppe giambarresi; David Gillan; Ruddy Wattiez; *Dept of Proteomic and Microbiology, UMONS, Mons, Belgium*
- MP 619 **PhosphoPath; Visualization of Phosphosite Specific Dynamics in Molecular Network Analysis of Large Phosphoproteomic Datasets;** Linsey Raaijmakers<sup>1</sup>; Piero Giansanti<sup>1</sup>; Patricia A. Possik<sup>2</sup>; Judith Mueller<sup>2</sup>; Daniel S. Peeper<sup>2</sup>; Albert J.R. Heck<sup>1</sup>; A.F. Maarten Altaar<sup>1</sup>; <sup>1</sup>Utrecht University, Utrecht, Netherlands; <sup>2</sup>Netherlands Cancer Institute, Amsterdam, Netherlands
- MP 620 **Monitoring Protein-Protein Interactions in Live Cells with a Wide Scope by Rapid Photo-Activated Cross-Linking and LC-MS/MS;** Anthony Persechini<sup>1</sup>; Boris Kornilayev<sup>1</sup>; Andrew Keightley<sup>1</sup>; Paul M Stemmer<sup>2</sup>; <sup>1</sup>Univ Missouri-Kansas City, Kansas City, MO; <sup>2</sup>Wayne State University, Detroit, MI
- MP 621 **Probing Paradoxical Effects of RAF Inhibition by Dynamic Phosphoproteomics;** Peter Kubiniok; H. Lavoie; M. Therrien; P. Thibault; *Universite de Montreal, Montreal, Canada*

- MP 622 **Quantitative Proteomic and Systems Analysis of Human Immune Cells in Response to Adjuvanted Influenza Vaccine**; Allison Galassie<sup>1</sup>; Parimal Samir<sup>2</sup>; Andrew Link<sup>1,2</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN Tennessee; <sup>2</sup>Vanderbilt University School of Medicine, Nashville, TN
- MP 623 **Global Analysis of Protein Folding Thermodynamics for the Characterization of Disease States**; Jagat Adhikari<sup>1</sup>; Graham West<sup>2,3</sup>; Michael C. Fitzgerald<sup>1</sup>; <sup>1</sup>Duke University, Durham, NC; <sup>2</sup>The Scripps Research Institute, Jupiter, FL; <sup>3</sup>Current Address: Pfizer, Inc, Groton, CT
- MP 624 **Pharmacoproteomic Analysis of the Resveratrol and DMSO**; Tanya Porras-Yakushi; Michael J Sweredoski; Sonja Hess; Caltech, Pasadena, CA
- MP 625 **Protease Inhibitors PZP and  $\alpha$ 2MG as Biochemical Keys to Find Unknown Mechanisms of Alzheimer's Disease**; Diana Nijholt; Peter Koudstaal; Arfan Ikram; Peter Sillevs-Smitt; Theo Luider; Erasmus Medical Centre, Rotterdam, The Netherlands
- MP 626 **A Systems Biology Approach for the Investigation of the Mechanism of Action of the Neurotrophic Drug Cerebrolysin**; Florian Füssli<sup>1</sup>; Stefan Winter<sup>2</sup>; Christian Huber<sup>1</sup>; <sup>1</sup>University of Salzburg, Salzburg, Austria; <sup>2</sup>Ever Neuro Pharma GmbH, Unterach, Austria
- MP 627 **Defining the Physical Interactome of the Active Kinome from the Intrinsic Subtypes of Human Breast Cancer**; Matthew R. Meyer<sup>1</sup>; Jing Wang<sup>3</sup>; Kelly V. Ruggles<sup>4</sup>; Petra Erdmann-Gilmore<sup>1</sup>; Jeanne Rumsey<sup>1</sup>; Robert Kitchens<sup>1</sup>; Jacqueline Snider<sup>1</sup>; Jeremy Hoog<sup>1</sup>; Shunqiang Li<sup>1</sup>; Sherri R. Davies<sup>1</sup>; Matthew J. Ellis<sup>2</sup>; David Fenyö<sup>4</sup>; Bing Zhang<sup>3</sup>; Gary L. Johnson<sup>5</sup>; R. Reid Townsend<sup>1</sup>; <sup>1</sup>Washington University School of Medicine, St. Louis, MO; <sup>2</sup>Baylor College of Medicine, Houston, TX; <sup>3</sup>Vanderbilt University, Nashville, TN; <sup>4</sup>New York University, New York, NY; <sup>5</sup>University of North Carolina, Chapel Hill, NC
- SYSTEMS BIOLOGY: OTHER**  
628 - 641
- MP 628 **Integrated Proteomics and Metabolomics Reveal Molecular Mechanism of Symbiotic Relationship between Fungal *Mortierella elongata* and Bacterial Endosymbiont *C. Glomeribacter* sp**; Zhou Li<sup>1</sup>; Stephen Dearth<sup>2</sup>; Qiuming Yao<sup>1</sup>; Jessie Uehling<sup>3</sup>; Hector Castro-Gonzalez<sup>2</sup>; Shawn Campagna<sup>2</sup>; Gregory Hurst<sup>1</sup>; Jessy Labbé<sup>1</sup>; Chongle Pan<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>University of Tennessee, Knoxville, TN; <sup>3</sup>Duke University, Durham, NC
- MP 629 **Discovering Metabolic Dynamics and Regulation by Real-Time Mass Spectrometry**; Tobias Fuhrer<sup>1</sup>; Hannes Link<sup>2</sup>; Andreas Kühne<sup>1</sup>; Uwe Sauer<sup>1</sup>; Nicola Zamboni<sup>1</sup>; <sup>1</sup>Institute of Molecular Systems Biology, ETH Zürich, Zürich, Switzerland; <sup>2</sup>Max Planck Institute for Terrestrial Microbiology, Marburg, Germany
- MP 630 **LC-MS/MS Characterization of the Microbiome Stability in Post-Surgery Crohn's Disease Patients**; J. Alfredo Blakeley-Ruiz<sup>1,2</sup>; Weili Xiong<sup>1,2</sup>; Robert Hettich<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>University of Tennessee, Knoxville, TN
- MP 631 **Studies of Heart Regeneration in Zebrafish: A Multi-Omics/System Biology Approach**; Leanne C. Nye<sup>1</sup>; Lee Gethings<sup>2</sup>; Cheng Shuk Han<sup>3</sup>; Yun Wah Lam<sup>3</sup>; Fatemeh Babaei<sup>3</sup>; Chi Chi Liu<sup>3</sup>; Alfred W. H. Chan<sup>3</sup>; Robert Plumb<sup>4</sup>; Ian D. Wilson<sup>1</sup>; <sup>1</sup>Imperial College, London, UK; <sup>2</sup>Waters Corporation, Wilmslow, UK; <sup>3</sup>City University, Hong Kong, Hong Kong; <sup>4</sup>Waters, Milford, MA
- MP 632 **Systematic Identification of the Lysine Succinylation in the Protozoan Parasite *Toxoplasma gondii***; Xiaolong Li<sup>2</sup>; Di Che<sup>3</sup>; Zhongyi Cheng<sup>1</sup>; Xingling Yi<sup>1</sup>; Feng Tan<sup>3</sup>; <sup>1</sup>PTM Biolabs, Inc, Hangzhou, China; <sup>2</sup>The First Affiliated Hospital of Wenzhou Medical U, Wenzhou, CN; <sup>3</sup>Wenzhou Medical University, Wenzhou, CN
- MP 633 **Systematic Integration Of "Omics" Data To Improve Innovation In Beer**; Barbara Dunn<sup>1</sup>; Dan Kvitcek<sup>2</sup>; Xiaoyue Jiang<sup>3</sup>; Daniel Lopez Ferrer<sup>3</sup>; Gina Tan<sup>3</sup>; Andreas Huhmer<sup>3</sup>; <sup>1</sup>Dept. of Genetics, Stanford University, Palo Alto, CA; <sup>2</sup>Invitae, San Francisco, CA; <sup>3</sup>Thermo Fisher Scientific, San Jose, CA
- MP 634 **LOPIT Proteomics Reveals Proteome-Wide Relocalisation upon Nitrogen Starvation in Yeast**; Daniel J. H. Nightingale<sup>1</sup>; Duygu Dikioglu<sup>2</sup>; Stephen G. Oliver<sup>2</sup>; Kathryn S. Lilley<sup>1</sup>; <sup>1</sup>Cambridge Centre for Proteomics, Cambridge, UK; <sup>2</sup>Cambridge Systems Biology Centre, Cambridge, UK
- MP 635 **Quantitative SWATH Proteomics Analysis of Tree-Fungal Interactions under Nutrient Limiting Conditions**; Landon Wilson<sup>1</sup>; Geetika Trivedi<sup>2</sup>; Avinash Sreedasyam<sup>3</sup>; Helen Kim<sup>1</sup>; Xiangqin Cui<sup>1</sup>; Leland J Cseke<sup>2</sup>; Stephen Barnes<sup>1</sup>; <sup>1</sup>University of Alabama at Birmingham, Birmingham, AL; <sup>2</sup>University of Alabama in Huntsville, Huntsville, AL; <sup>3</sup>HudsonAlpha Institute for Biotechnology, Huntsville, AL
- MP 636 **Towards High-Throughput Analysis of Salmonella Serotypes: A Fundamental Look at Protein Profiles, Proteomes and Secretomes of *Salmonella typhimurium* and *enteritidis***; Amornmart Jaratrungratawee<sup>1</sup>; Jaran Jainhuknan<sup>1</sup>; Saw Yen Ow<sup>2</sup>; Onrapak Reamtong<sup>3</sup>; Tipparat Thiangtrongjit<sup>3</sup>; Yuphakhun Chaturongkasumrit<sup>4</sup>; Mongkol Vesaratchavest<sup>4</sup>; <sup>1</sup>Bruker Corporation, Bangkok, Thailand; <sup>2</sup>Bruker Corporation, Kuala Lumpur, Malaysia; <sup>3</sup>Mahidol University, Bangkok, Thailand; <sup>4</sup>Research and Development Center, Betagro Group, Bangkok, Thailand
- MP 637 **Enhanced Informatics Methods for Integrating Metagenome and Metaproteome Information for the Pre-term Human Gut Microbiome**; Robert Hettich<sup>1</sup>; Weili Xiong<sup>1,2</sup>; Alison Erickson<sup>1</sup>; J.J. Chai<sup>1</sup>; Chongle Pan<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>University of Tennessee, Knoxville, TN
- MP 638 **Quantitative Proteomic Analysis Reveals Environmental Interaction and Epistasis in the Responses to Complex Stimuli in *Saccharomyces cerevisiae***; Parimal Samir<sup>1</sup>; Rahul<sup>2</sup>; Andrew Link<sup>1</sup>; <sup>1</sup>Vanderbilt University School of Medicine, Nashville, TN; <sup>2</sup>University of Waterloo, Waterloo, Canada
- MP 639 **Proteome-in-motion: Deep Study of Protein Dynamics and Regulation in Yeast Proliferating Cells**; Miguel Martin Perez; Judit Villen; University of Washington, Seattle, WA
- MP 640 **Comprehensive Quantitation of 1,000 Proteomes**; Alicia L. Richards; Alexander S. Hebert; Jonathan A. Stefely; Elyse C. Freiburger; Nicholas W. Kwiecien; Adam Jochem; Xiao Guo; Michael S. Westphal; David J. Pagliarini; Joshua J. Coon; University of Wisconsin, Madison, WI
- MP 641 **Proteomic Visualization of Nanoparticle Cellular Entry Pathways**; Linna Wang; Li Yang; Naveen Kadasala; Li Pan; Alexander Wei; Weiguo Andy Tao; Purdue University, West Lafayette, IN
- ENERGY: HYDROCARBON AND PETROCHEMICAL**  
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- MP 642 **Correlation of Boiling Point, Molecular Weight and Composition by Mass Spectrometry: The Development of Class Dependent Equations**; Yuri E. Corilo<sup>1,2</sup>; Priscila M. Lalli<sup>2</sup>; Steven M. Rowland<sup>2</sup>; Logan C. Krajewski<sup>1</sup>; Alan G. Marshall<sup>1,3</sup>; Ryan P. Rodgers<sup>1</sup>; <sup>1</sup>National High Magnetic Field Laboratory, FSU, Tallahassee, FL; <sup>2</sup>Future Fuels Institute, FSU, Tallahassee, FL; <sup>3</sup>Department of Chemistry and Biochemistry, FSU, Tallahassee, FL
- MP 643 **Structural Identification of Naphthyl Compounds in 2,6-naphthalenedicarboxylic Acid by UPLC-QTOF Tandem Mass Spectrometry**; Junyan Liu; Liyan Jiang; Sinopec Shanghai Research Institute of Petrochem, Shanghai, China



- MP 644 **Probing Nanoaggregation of Asphaltene Model Compound using Electrospray Ionization Mass Spectrometry;** Lan Liu<sup>1</sup>; Johan Sjöblom<sup>2</sup>; Zhenghe Xu<sup>1</sup>; <sup>1</sup>University of Alberta, Edmonton, Canada; <sup>2</sup>Norwegian University of Science and Technology, Trondheim, Norway
- MP 645 **Comprehensive Characterization of Petroleum – Crude Oil, Asphaltenes and Sulfur Compounds;** Jeffrey Patrick; Joe Binkley; Jonathan Byer; Clécio Klitzke; *LECO Corporation, St. Joseph, MI*
- MP 646 **Characterization of Semi-Synthetic Motor Oil using FT-ICR;** Sung Hwan Yoon; David Goodlett; David Kilgour; *University of Maryland, Baltimore, MD*
- MP 647 **Study of Asphaltene Adsorption on Mineral Surfaces by High-Resolution Mass Spectrometry;** Martha Chacón-Patiño<sup>1</sup>; José J. Villarreal<sup>1</sup>; Andrea Gomez-Escudero<sup>2</sup>; Jorge A. Orrego-Ruiz<sup>2</sup>; Cristian Blanco-Tirado<sup>1</sup>; Marianny Y. Combariza<sup>1</sup>; <sup>1</sup>UIS, Bucaramanga, Colombia; <sup>2</sup>ECOPETROL, Piedecuesta Santander
- MP 648 **Identification of Challenging Components in Complex Hydrocarbon Mixtures using High Resolution GC/Q-TOF with an Innovative EI Source;** Pierre Giusti<sup>1</sup>; Sabrina Marceau<sup>1</sup>; Benoit Paupy<sup>1</sup>; Sofia Nieto<sup>2</sup>; Mingda Wang<sup>2</sup>; Harry Prest<sup>2</sup>; <sup>1</sup>TOTAL Refining and Chemicals, TRTG, Gonfreville l'Orcher, France; <sup>2</sup>Agilent Technologies, Inc., Santa Clara, CA
- MP 649 **MS/MS of Aromatic Surfactants, Structure Determination of Mixture by Charge Remote Fragmentation at High Resolving Power;** Michael T. Cheng<sup>1</sup>; Matthew Hurt<sup>2</sup>; <sup>1</sup>Chevron Research, Richmond, CA; <sup>2</sup>Chevron, Richmond, CA
- MP 650 **Application of Design of Experiment (DOE) and Optimization by Atmospheric Pressure Photoionization (APPI) Source Parameters for Studies in Petroleomics;** Jandysom Machado Santos<sup>1</sup>; Marcos A. Pudenzi<sup>1</sup>; Eduardo M. Schmidt<sup>1</sup>; Heliara D. L. Nascimento<sup>1</sup>; Alberto Wisniewski Jr.<sup>2</sup>; Marcos N. Eberlin<sup>1</sup>; <sup>1</sup>University of Campinas, Campinas, SP; <sup>2</sup>Federal University of Sergipe, São Cristóvão, SE
- MP 651 **Supercritical Fluid Chromatography Coupled with Ion Mobility-Mass Spectrometry for Comprehensive Profiling of Petroleum Samples;** Eleanor Riches<sup>1</sup>; Yunju Cho<sup>2</sup>; Sunghwan Kim<sup>2</sup>; <sup>1</sup>Waters Corporation, Wilmslow, UK; <sup>2</sup>Chemistry Department, Kyungpook National University, Daegu, South Korea
- MP 652 **Characterization of Heteroatom-Containing Species in Lignite with Orbitrap Mass Spectrometry and Statistical Analysis;** Lu Chen; Xing Fan; Chun-Yan You; Xian-Yong Wei; Yun-Peng Zhao; Jun-Liu Xia; Miao Wang; *China University of Mining & Technology, Xuzhou, China*
- MP 653 **Analysis of Dibenzothiophenes in Diesel by GC-APCI Ion Mobility High Resolution Mass Spectrometry;** Sheher Bano Mohsin<sup>1</sup>; David Wong<sup>2</sup>; Robert Ley<sup>2</sup>; <sup>1</sup>Agilent Technologies, Schaumburg, IL; <sup>2</sup>Agilent Technologies, Inc., Santa Clara, CA
- MP 654 **Standard Compounds Analysis as a Tool for the Establishment of Ionization/Intrinsic Characteristics Relationship on Crude Oil Polar Compounds;** Marcos Albieri Pudenzi<sup>1</sup>; Clécio Fernando Klitzke<sup>1</sup>; Vanessa Gonçalves Santos<sup>1</sup>; Heliara D. Lopes Nascimento<sup>1</sup>; Pedro Henrique Vendramini<sup>1</sup>; Eduardo Morgado Schmidt<sup>1</sup>; Rosana Cardoso Lopes Pereira<sup>2</sup>; Wagner Leonel Bastos<sup>2</sup>; Marcos Nogueira Eberlin<sup>1</sup>; <sup>1</sup>Unicamp, Campinas, Brasil; <sup>2</sup>CENPES, PETROBRAS, Rio de Janeiro, RJ - Brasil
- MP 655 **Application of Molecular Dynamic Simulation for More Accurate CCS Calculations of Aromatic Compounds with Long Alkyl Chains;** Arif Ahmed<sup>1</sup>; Dongwan Lim<sup>1</sup>; Jong Wha Lee<sup>2</sup>; Hugh I. Kim<sup>2</sup>; Sunghwan Kim<sup>1,3</sup>; <sup>1</sup>Kyungpook National University, Daegu, Republic of Korea; <sup>2</sup>Pohang University of Science and Technology, Pohang, Republic of Korea; <sup>3</sup>Green-Nano Materials Research Center, Daegu, Republic of Korea
- MP 656 **Comparison of Interface-Active Materials in Crude Oils with Different Emulsifying Propensities by using Solid Phase Extraction and an LTQ-Obitrap Mass Spectrometer;** Xueming Dong; Chunfen Jin; Ravikiran Yerabolu; Hiikka Kenttamaa; *Purdue University, West Lafayette, IN*
- MP 657 **Nitrogen Speciation in Petroleum Distillates using a Complementary and Powerful Approach by GC×GC-NCD and FT-ICR/MS;** Fabien Chainet; Lyes Assam; Vincent Souchon; Jérémie Ponthus; Florian Albrieux; *IFPEN, Solaize, France*
- MP 658 **A Model Compound Study to Assess Potential Complications of Using APPI for Mass Spectrometric Analysis of Crude Oil;** Matthew Hurt; Michael T. Cheng; *Chevron Research, Richmond, CA*
- MP 659 **Pretreatment of Oil Samples for GCMS Analysis of Polycyclic Aromatic Hydrocarbons and Their Hetero-Analogs;** Nino Todua<sup>1</sup>; Natela Khetsuriani<sup>2</sup>; Elza Topuria<sup>2</sup>; Levan Megutnishvili<sup>1</sup>; Alexey Mayorov<sup>1</sup>; Anzor Mikaia<sup>1</sup>; <sup>1</sup>National Institute of Standards & Technology, Gaithersburg, MD; <sup>2</sup>Melikhishvili Institute of Phys. & Org. Chemistry, Tbilisi, Georgia
- MP 660 **Development of an Analytical Method for Complex Downstream Hydrocarbons of Gas Cracker by GC/GC-MS;** Syed Ali; Asraf Ali; Momdoh Al-Enzi; Ibrahim Al-Ghamdi; Nasser M. Al-Harbi; Khalid H. Al-Assaf; *SABIC Research Center, Riyadh, Saudi Arabia*
- MP 661 **Analysis of Complex Aromatic Mixtures Such as Asphaltenes using Online Coupling LC-MS Methods;** Lilla Molnárné Guricza; Schrader Wolfgang; *Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany*
- MP 662 **Characterization of Isomers in Petroleum Interfacial Material by Ion Mobility Mass Spectrometry;** Priscila M. Lalli<sup>1,2</sup>; Jacqueline M. Jarvis<sup>1</sup>; Alan G. Marshall<sup>1,3</sup>; Ryan P. Rodgers<sup>1,2</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>Florida State University Future Fuels Institute, Tallahassee, FL; <sup>3</sup>Department of Chemistry, Florida State University, Tallahassee, FL
- MP 663 **Analysis of Naphthenic acids by Matrix Assisted Laser Desorption Ionization Time of Flight Mass Spectrometry;** Jeferson Valencia; Marianny Yajaira Combariza; Cristian Blanco Tirado; *Universidad Industrial de Santander, Bucaramanga, Colombia*
- MP 664 **Unprecedented Inventory of Coal Tar Compounds by an Integrative Approach Comprising GCxGC-TOF MS and APPI(+)-FT-ICR MS;** Hector Koolen<sup>1</sup>; Robert Swarthout<sup>1</sup>; Robert Nelson<sup>1</sup>; Huan Chen<sup>2</sup>; Logan Krajewski<sup>2</sup>; Christoph Aeppli<sup>3</sup>; Amy McKenna<sup>2</sup>; Ryan Rodgers<sup>2</sup>; Christopher Reddy<sup>1</sup>; <sup>1</sup>Woods Hole Oceanographic Institution, Woods Hole, MA; <sup>2</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>3</sup>Bigelow Laboratory for Ocean Sciences, East Boothbay, ME
- MP 665 **Evaluation of Biodegradation of Crude Oils by Gcxcg using New Strategies Chemometrics;** Paloma Santana Prata; Noroska Gabriela Salazar Mogollón; Fabio Augusto; *Unicamp, Campinas, BR*
- MP 666 **Determination of Molecular Changes in Asphaltene Composition during Hydroconversion and Thermal Cracking Processes by High Resolution Mass Spectrometry;** Martha L. Chacón-Patiño<sup>1</sup>; Cristian Blanco-Tirado<sup>1</sup>; Jorge A. Orrego-Ruiz<sup>2</sup>; Andrea Gómez-Escudero<sup>2</sup>; Marianny Y. Combariza<sup>1</sup>; <sup>1</sup>Universidad Industrial de Santander, Bucaramanga, Colombia; <sup>2</sup>Instituto Colombiano del Petróleo, Piedecuesta, Colombia

## CARBOHYDRATES I

667 - 692

- MP 667 **Evaluation of the INLIGHT™ strategy for LC-MS/MS Disaccharide Analysis;** Adam Hawkrigde; John Mangrum; Umesh Desai; *Virginia Commonwealth University, Richmond, VA*
- MP 668 **Development of Bioinformatics Support for High Throughput Isomeric Separation and the Structural Identification of Glycans by LC-MS;** Ningombam Sanjib Meitei<sup>1</sup>; Arun Apte<sup>2</sup>; Udayanath Aich<sup>3</sup>; Julian Saba<sup>4</sup>; <sup>1</sup>PREMIER Biosoft, Indore, India; <sup>2</sup>PREMIER Biosoft, Palo Alto, CA; <sup>3</sup>Thermo Fisher Scientific, Sunnyvale, CA; <sup>4</sup>Thermo Fisher Scientific, San Jose, CA
- MP 669 **Intelligent Glycomics Data-Independent-Acquisition Method (iGODIA) for Targeted Glycotope Analysis;** Hsin-Hung Huang<sup>1,2</sup>; Kay-Hooi Khoo<sup>1,2</sup>; <sup>1</sup>IBC, Academia Sinica, Taipei, Taiwan; <sup>2</sup>IBS, National Taiwan University, Taipei, Taiwan
- MP 670 **MultiGlycan: A Software Tool for Automated Glycan Quantification using Labeling-Based and Label Free Approaches;** Chuan-Yih Yu<sup>1</sup>; Yunli Hu<sup>2</sup>; Shiyue Zhou<sup>2</sup>; Yehia Mechref<sup>2</sup>; Haixu Tang<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN; <sup>2</sup>Texas Tech University, Lubbock, TX
- MP 671 **Development of Structural Analysis Techniques for Keratan Sulfate Using Chemical Derivatization and LC-MS/MS;** David Fischler; *Complex Carbohydrate Research Center, UGA, Athens, GA*
- MP 672 **Towards Absolute Quantification in Glycomics Facilitating New Labeling Strategies for *Pichia pastoris* N-glycans;** Evelyn Rampler; Gunda Koellensperger; *University Vienna, Vienna, Austria*
- MP 673 **Using an Isotopically Labelled Glycoprotein Internal Standard to Enable Comparison of Glycan Quantitation across Mass Spectrometer Types;** Emily Betchy<sup>1</sup>; Barry Boyes<sup>2</sup>; Ron Orlando<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA; <sup>2</sup>Advanced Materials Technology, Wilmington, DE
- MP 674 **Towards the Discrimination of Sialyl Linkages in Glycopeptides: A New Derivatization Approach;** Takashi Nishikaze; Shinichi Iwamoto; Koichi Tanaka; *Shimadzu Corporation, Kyoto, Japan*
- MP 675 **Semi-Automatic Site Specific Analysis of High Mannose and Hybrid Type Glycosylation of Human Serum Glycoproteins in Liver Disease;** Miloslav Sanda<sup>1</sup>; Nathan J Edwards<sup>2</sup>; Radoslav Goldman<sup>1</sup>; <sup>1</sup>Department of Oncology, Lombardi Comprehensive, Washington, DC; <sup>2</sup>Department of Biochemistry and Molecular & Cell, Washington, DC
- MP 676 **Survey of Cationizing Metals for CID and ETD of Metal-Adducted Oligosaccharides;** Ranelle M. Schaller-Duke; Carolyn J. Cassidy; *The University of Alabama, Tuscaloosa, AL*
- MP 677 **Determination of Caulobacter Crescentus Glycan Strand Length Distribution by LC-UV-MS;** Ludmila Alexandrova<sup>1</sup>; Allis Chien<sup>1</sup>; Leigh Harris<sup>2</sup>; Julie Theriot<sup>2</sup>; <sup>1</sup>Stanford University Mass Spectrometry, Stanford, CA; <sup>2</sup>Biophysics Program, Department of Biochemistry, Stanford, CA
- MP 678 **Rapid Characterization of Model Glycosaminoglycans using Negative Electron Transfer Dissociation;** Matthew Rush; Nicholas Riley; Christopher Rose; Alexander Hebert; Michael Westphall; Joshua Coon; *University of Wisconsin, Madison, WI*
- MP 679 **Electrospray Ionization of Saccharides by Amino Acids;** Abdil Ozdemir<sup>2</sup>; Chung-Hsuan Chen<sup>1</sup>; <sup>1</sup>Academia Sinica, Genomics Research Center, Taipei, Taiwan; <sup>2</sup>Sakarya University, Adapazari, Turkey
- MP 680 **Mass Spectrometric Analysis to Identify arabino-xylo-oligomers Generated from Hydrothermal Processing Of Switchgrass;** Michael Bowman; Victoria Nguyen; Bruce Dien; *USDA-NCAUR, Peoria, IL*
- MP 681 **The Coolest Sugars in the Universe: Characterizing Complex Carbohydrates in Liquid Helium Nanodroplets;** Christiane Stachl<sup>1</sup>; Ana Isabel González Flórez<sup>1</sup>; Doo-Sik Ahn<sup>1</sup>; Johanna Hofmann<sup>1</sup>; Heung Sik Hahn<sup>2</sup>; Peter Seeberger<sup>2</sup>; Gert von Helden<sup>1</sup>; Kevin Pagel<sup>1</sup>; <sup>1</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany; <sup>2</sup>Max Planck Institute of Colloids and Interfaces, Potsdam, Germany
- MP 682 **Reliable Quantitative Glycomics using LC-MS and iGlycoMab Stable Isotope Labeled Glycan Standard;** Nadia Tello<sup>1</sup>; Shiyue Zhou<sup>1</sup>; Alex Harvey<sup>2</sup>; Barry Boyes<sup>2</sup>; Ron Orlando<sup>2</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>Texas Tech University, Lubbock, TX; <sup>2</sup>GlycoScientific, Athens, GA
- MP 683 **Addition of Basic Sites to the Glycans of *Helicobacter pylori* to Increase MS/MS Peak Abundance;** Haley S. Miller; Danielle Dube; Elizabeth A. Stemmler; *Bowdoin College, Brunswick, ME*
- MP 684 **Improved Sensitivity in Tandem MS Quantification of Heparan Sulphate by Depolymerisation Using Acid Butanolysis Reaction;** Paul J Trim; John Hopwood; Marten Snel; *South Australian Health and Medical Research Insti, Adelaide, Australia*
- MP 685 **Analysis of Fructosylamino Acids in Dried Fruit Utilizing Deuterated *n*-butyl-ketoximes as Standards by Gas-Liquid Chromatography/Mass Spectrometry;** Thomas P. Mawhinney; Deborah Chance; Valeri Mossine; Brock Evans; Carl Cheadle; James Waters; *University of Missouri, Columbia, MO*
- MP 686 **Quantification and Structural Characterization of Glycans and Glycopeptides by TQMS: The Energy-Resolved Oxonium Ion Monitoring (Erexim) Platform;** Atsuhiko Toyama<sup>1</sup>; Shuichi Nakaya<sup>1</sup>; Shinji Funatsu<sup>1</sup>; Koji Ueda<sup>2</sup>; Yoshihiro Hayakawa<sup>1</sup>; Ichiro Hirano<sup>1</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>The University of Tokyo, Tokyo, Japan
- MP 687 **Branched Oligosaccharides by Microwave Assisted Hydrolysis, HILIC Separation, and MS<sup>n</sup> (n>2);** Jia Ren; *Purdue University, West Lafayette, IN*
- MP 688 **Esterification of Glycopeptides for the Determination of Sialylation Levels in Antibodies;** Andrey Oliveira<sup>1</sup>; Rini Roy<sup>1</sup>; Paul Lopez<sup>1</sup>; Edward Bodnar<sup>1</sup>; Celine Raymond<sup>2</sup>; Yves Durocher<sup>2</sup>; Helene Perreault<sup>1</sup>; <sup>1</sup>University of Manitoba, Winnipeg, Canada; <sup>2</sup>National Research Council of Canada, Montreal, Qc
- MP 689 **LC-MS/MS Analysis of Permethylated Free Oligosaccharides and N-glycans Released from Human Milk;** Xue Dong; Shiyue Zhou; Nadia Tello; Yehia Mechref; *Texas Tech University, Lubbock, TX*
- MP 690 **Mass Spectral Patterns Obtained by Field Ionization GC/MS of Methyloxime-TMS-derivatized Primary Metabolites;** Takeshi Furuhashi<sup>1</sup>; Takemichi Nakamura<sup>2</sup>; <sup>1</sup>RIKEN, Yokohama, Japan; <sup>2</sup>RIKEN, Wako, Japan
- MP 691 **Advanced LC-MS Based Approaches for Orthogonal Determination of N- and O-linked Glycosylation Structures in Therapeutic Proteins;** Chen Li<sup>1</sup>; Peter Li<sup>1</sup>; Douglas Richardson<sup>2</sup>; Huijuan Li<sup>2</sup>; Yuetian Chen<sup>2</sup>; Daisy Richardson<sup>2</sup>; Mohammed Shameem<sup>2</sup>; David Pollard<sup>2</sup>; Shiao-Lin Wu<sup>1</sup>; <sup>1</sup>BioAnalytix, Cambridge, MA; <sup>2</sup>Merck & Co, Kenilworth, NJ
- MP 692 **Heparan Sulfate Libraries Derived From Robo-1 Affinity Pulldowns;** Morgan Stickney<sup>1</sup>; David Fischler<sup>2</sup>; Rongrong Huang<sup>2</sup>; Joshua S. Sharp<sup>2</sup>; Jon Amster<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA; <sup>2</sup>Complex Carbohydrate Research Center, UGA, Athens, GA



These special posters will be displayed Monday through Thursday.

Special **IPRG 2015 Study: Differential Abundance Analysis in Label-free Quantitative Proteomics**; Eugene Kapp<sup>7</sup>; Henry Lam<sup>10</sup>; Brett Phinney<sup>2</sup>; John S. Cottrell<sup>3</sup>; Michael R. Hoopmann<sup>4</sup>; Sangtae Kim<sup>8</sup>; Thomas Neubert<sup>5</sup>; Magnus Palmblad<sup>6</sup>; Olga Vitek<sup>9</sup>; Susan T. Weintraub<sup>1</sup>; <sup>1</sup>Univ. of Texas HSC, San Antonio, TX; <sup>2</sup>Univeristy of CA, Davis, Davis, CA; <sup>3</sup>Matrix Science, Ltd., London, UK; <sup>4</sup>Institute for Systems Biology, Seattle, WA; <sup>5</sup>Skirball Institute, NYUMC, New York, NY; <sup>6</sup>Leiden University, Leiden, Netherlands; <sup>7</sup>Walter and Eliza Hall Institute of Medical Researc, Parkville, Australia; <sup>8</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>9</sup>Northeastern University, Boston, MA; <sup>10</sup>Hong Kong University of Science and Technology, Hong Kong, Hong Kong

Special **Mapping Scientific Pedigrees and Collaborative Patterns using Bibliometrics: Six Former Presidents of the ASMS**; Arzu Tugce Guler<sup>1</sup>; Cathelijm Waaaijer<sup>2</sup>; Magnus Palmblad<sup>1</sup>; <sup>1</sup>Leiden University Medical Center, Leiden, Netherlands; <sup>2</sup>Leiden University, Leiden, Netherlands

TUESDAY POSTERS

7:30 – 8:00 am.....	Set up all Tuesday posters	Environmental Analysis: Pharmaceuticals and Pesticides .....	296-323
10:30 am – 1:00 pm.....	Odd-numbered posters present	Food Safety .....	324-355
12:00 – 2:30 pm.....	Even-numbered posters present	Microorganisms: Identification and Characterization.....	356-370
7:30 – 8:00 pm.....	Remove all Tuesday posters	H/D Exchange: Protein Structure/Function.....	371-384
Ambient Ionization: Application.....	001-028	Top Down Protein Analysis: Complex Sample LC-MS .....	385-403
Ion Spectroscopy.....	029-038	Proteins: General.....	404-423
Ion/Molecule, Ion/Ion, Ion/Electron Interactions .....	039-060	Glycoproteins: Complex Samples .....	424-448
Instrumentation: General.....	061-079	Proteins: Phosphoproteins .....	449-462
Instrumentation: New Developments in Ionization		Proteins: Membrane .....	463-472
and Sampling.....	080-099	Proteins: Complexes .....	473-494
High Mass Accuracy/High Performance MS: Applications .....	100-117	Protein Therapeutics: Structural Characterization.....	495-513
High Mass Accuracy/High Performance MS: Instrumentation..	118-126	Proteomics: Infectious Disease .....	514-529
Informatics: Workflow and Data Management.....	127-140	Proteomics: New Approaches - Innovative Methods.....	530-555
Data Independent Acquisition.....	141-163	Proteomics: New Approaches - Sample Preparation	
Metabolomics: Untargeted Metabolite Profiling I.....	164-193	Methods.....	556-586
Metabolomics: Untargeted Metabolite Profiling II.....	194-218	Proteomics: Quantitative - Stable Isotope Labeling Methods...587-605	
Drug Metabolism: Qualitative Analysis .....	219-234	Biomarker: Quantitative Analysis (non-protein, lipids/metabolites/	
Lipidomics: New Technologies .....	235-245	compounds).....	606-629
Lipids: General .....	246-260	Disease Biomarkers .....	630-654
Lipids: Profile Analysis and Lipidomics.....	261-276	Imaging MS: Pharmaceutical Applications .....	655-667
Small Molecules: Quantitative Analysis.....	277-295	Imaging MS: Disease Markers .....	668-694

AMBIENT IONIZATION: APPLICATION  
001-028

TP 001	<b>Optimization and Application of Continuous Solvent Addition and Controlled Elution to Paper Spray Ionization</b> ; Elizabeth Dhummakupt; Michael Wei; Richard A. Yost; <i>University of Florida, Gainesville, FL</i>	TP 006	<b>Thermal Gravimetric Analysis Coupled with Ambient Mass Spectrometry (TG-AMS) for Rapid Determination of Chemical Components in Plastic and Rubber Products</b> ; Siou Sian Jhang; Min Zong Huang; Jentaie Shiea; <i>National Sun Yat- Sen University, Kaohsiung, Taiwan</i>
TP 002	<b>Characterization of Sterols in Vegetable Oils by Transmission Mode Direct Analysis in Real Time Mass Spectrometry</b> ; Rosana Alberici <sup>1</sup> ; Gabriel Fernandes <sup>2</sup> ; Andréia Porcari <sup>1</sup> ; Marcos Eberlin <sup>1</sup> ; Daniel Barrera-Arellano <sup>2</sup> ; Facundo Fernandez <sup>2</sup> ; <sup>1</sup> Thomson Mass Spectrometry Laboratory-UNICAMP, Campinas, Brazil; <sup>2</sup> Fats and Oils Laboratory-UNICAMP, Campinas, Brazil; <sup>3</sup> Georgia Institute of Technology, Atlanta, GA	TP 007	<b>Ambient Analysis of Leachable Compounds from Single-Use Bioreactors with Desorption Electrospray Ionization Time-of-Flight Mass Spectrometry</b> ; Jian Liu <sup>1</sup> ; Joseph H Kennedy <sup>2</sup> ; Mike Ronk <sup>1</sup> ; Liliana Marghitoiu <sup>1</sup> ; Hans Lee <sup>1</sup> ; Yasser Nashed-Samuel <sup>1</sup> ; <sup>1</sup> Amgen, Thousand Oaks, California; <sup>2</sup> Prosolia, Inc., Indianapolis, IN
TP 003	<b>Direct Analysis in Real Time-Mass Spectrometry (DART-MS) for the Study of Gas-Surface Heterogeneous Reactions: Focus on Ozone and PAHs</b> ; Shouming Zhou; Matthew W. Forbes; Jonathan P.D. Abbatt; <i>Department of Chemistry, University of Toronto, Toronto, Canada</i>	TP 008	<b>Gas Chromatography Coupled with ESI/APCI Dual Ion Source for Simultaneous Detection of Polar and Nonpolar Compounds</b> ; Ban Hsin Wu; Siou Sian Jhang; Min Zong Huang; Jentaie Shiea; <i>National Sun Yat-Sen Univ., Kaohsiung, Taiwan</i>
TP 004	<b>Continuous-Wavelength Laser Desorption Coupled with ESI/APCI Dual Ion Source for Rapid Characterization of Packaging Materials</b> ; Yi Lun Chen; Siou Sian Jhang; Min Zong Huang; Jentaie Shiea; <i>National Sun Yat- Sen University, Kaohsiung, Taiwan</i>	TP 009	<b>Using DART Mass Spectrometry for an Undergraduate Analytical Chemistry Laboratory</b> ; Nathan Cunningham; Hong Hanh Nguyen; Joseph A. Loo; <i>UCLA, Los Angeles, CA</i>
TP 005	<b>Direct Analysis from TLC Plate using Matrix Assisted Ionization (MAI)</b> ; Khoa Hoang; Charles McEwen; , <i>Philadelphia, PA</i>	TP 010	<b>Rapid, Direct Technique for the Discrimination of Meat Tissues Originating from Different Animal Species for Food Authenticity</b> ; Sara Stead; Simon Hird; Julia Balog; Alex Hooper; Steve Pringle; Mike Wilson; Mike Morris; <i>Waters corp, Manchester, UK</i>

- TP 011 **Integration of GC/LC with ESI+APCI/MS for Analysis of Complicated Mixtures over a Wide Polarity Range;** Sy chyi Cheng; Siou Sian Jhang; Min Zong Huang; Jentaie Shiea; *National Sun Yat-Sen Univ., Kaohsiung, Taiwan*
- TP 012 **Direct Quantitative Analysis of Drugs of Abuse in Urine and Saliva;** Chris Hopley; Bryan McCullough; Camilla Liscio; *LGC, Teddington, UK*
- TP 013 **Liquid Microextraction Coupled with Thermal Desorption Electrospray Ionization Mass Spectrometry for Rapid Screening of Veterinary Drug Residues in Foods;** Peng Yu Chen; Jo Han Chou; Min Zong Huang; Jentaie Shiea; *National Sun Yat-Sen University, Kaohsiung, Taiwan*
- TP 014 **Mobile Screening of Glycerin Contaminants using Paper Spray Portable Mass Spectrometry;** Samanthi I. Wickramasekara; Hongli Li; Dinesh Patwardhan; Steven Wolfgang; *US Food and Drug Administration, Silver Spring, MD*
- TP 015 **Rapid Differentiation of Ganoderma Species by Direct Ionization Mass Spectrometry;** Ho-Yi Wong; Bin Hu; Pui-Kin So; Chi-On Chan; Daniel Kam-Wah Mok; Zhong-Ping Yao; *Department of Applied Biology & Chemical Technology, The Hong Kong Polytechnic University, Hong Kong*
- TP 016 **Molecular Analyses of Algae using Desorption Electrospray Ionization (DESI) and Laser Desorption/Ionization (LDI) Mass Spectrometry;** Dilrukshika S. W. Palagama; Raymond E. West III; Dragan Isailovic; *The University of Toledo, Toledo, OH*
- TP 017 **Desorption Ionization of Illicit Drugs from Solid Phase Micro-Extraction Fibers at Increasing Temperature;** Joseph Lapointe<sup>1</sup>; Brian Musselman<sup>1</sup>; Craig Aurand<sup>2</sup>; <sup>1</sup>*Ionsense Inc., Saugus, MA*; <sup>2</sup>*Sigma Aldrich, Bellefonte, PA*
- TP 018 **Defining Limit of Detection of Mini Surface Acoustic Wave Nebulization Chip by Using Different Types of Mass Spectrometer;** Tao Liang<sup>1</sup>; Andrew Dennison<sup>2</sup>; Sung Hwan Yoon<sup>1</sup>; Gloria Yen<sup>5</sup>; Yifan Li<sup>4</sup>; Scott Heron<sup>1</sup>; Adam Stokes<sup>3</sup>; Anthony Walton<sup>2</sup>; Erik Nilsson<sup>5</sup>; David Goodlett<sup>1</sup>; <sup>1</sup>*Pharmacy School, University of Maryland Baltimore, Baltimore, MD*; <sup>2</sup>*School of Chemistry, The University of Edinburgh, Edinburgh, UK*; <sup>3</sup>*School of Engineering, The University of Edinburgh, Edinburgh, UK*; <sup>4</sup>*Department of Engineering, Northumbria University, Newcastle, UK*; <sup>5</sup>*Deurion LLC, Seattle, WA*
- TP 019 **Rapid Screening and Identification of Designer Drugs in Powders or Plant Materials using Paper Spray Ionization-Mass Spectrometry;** Joseph H Kennedy<sup>1</sup>; Kevin G. Shanks<sup>2</sup>; Justin Wiseman<sup>1</sup>; Brian C. Laughlin<sup>1</sup>; <sup>1</sup>*Prosolia, Inc., Indianapolis, IN*; <sup>2</sup>*AIT Laboratories, Indianapolis, IN*
- TP 020 **Thermal Desorption Electrospray Ionization Mass Spectrometry Combined with Principal Component Analysis for Rapid Classification of Cooking Oils;** Ting Hao Chang; Siou Sian Jhang; Min Zong Huang; Jentaie Shiea; *National Sun Yat-Sen University, Kaohsiung, Taiwan*
- TP 021 **Using Desorption Electrospray Ionization with Mass Spectrometry (DESI-MS) to Identify Silicone Oil Contamination on Components;** Lance Miller; James Hochrein; *Sandia National Laboratories, Albuquerque, NM*
- TP 022 **DART-MS Determination of Malachite Green and Leucomalachite Green in Fish Extract;** Jia Shi<sup>1</sup>; Xiaokun Duan<sup>2</sup>; Kai Liu<sup>2</sup>; Charles C. Liu<sup>2</sup>; Hongwei Zhao<sup>3</sup>; <sup>1</sup>*Sichuan Aquaculture Bureau, Chengdu, Sichuan*; <sup>2</sup>*ASPEC Technologies LTD, Beijing, China*; <sup>3</sup>*Xiangpu Technology, Chengdu, Sichuan*
- TP 023 **In situ Detection and Imaging of Ergot Alkaloids in Ipomoea tricolor Seeds by LAESI-MS/MS;** Gregory Boyce<sup>1</sup>; Callee Walsh<sup>1</sup>; Daniel Panaccione<sup>2</sup>; <sup>1</sup>*Protea Biosciences, Morgantown, WV*; <sup>2</sup>*West Virginia University, Morgantown, WV*
- TP 024 **A Continuous Microplasma-Coupled Sampling Device for Real-Time Monitoring of Environmental Quality during Space Missions;** Matthew C. Bernier<sup>1</sup>; Joel D. Keelor<sup>1</sup>; Rosana M. Alberici<sup>2</sup>; Prabha Dwivedi<sup>1</sup>; Daniel B. Gazda<sup>3</sup>; Thomas F. Limerio<sup>3</sup>; William T. Wallace<sup>3</sup>; Ariel V. Macatangay<sup>4</sup>; Joshua M. Symonds<sup>1</sup>; Thomas M. Orlando<sup>1</sup>; Facundo M. Fernandez<sup>1</sup>; <sup>1</sup>*Georgia Institute of Technology, Atlanta, GA*; <sup>2</sup>*Thomson Mass Spectrometry Laboratory, UNICAMP, Campinas, Brazil*; <sup>3</sup>*Wyle Science, Technology, and Engineering Group, Houston, TX*; <sup>4</sup>*NASA Johnson Space Center, Houston, TX*
- TP 025 **Monolayer-Coated Probe Electrospray Ionization Mass Spectrometry for Analysis of Individual Small Organisms and Single Cells;** Jiewei Deng<sup>1</sup>; Yunyun Yang<sup>2</sup>; Mingzhi Xu<sup>1</sup>; Xiaowei Wang<sup>1</sup>; Zhong-Ping Yao<sup>3</sup>; Tiangang Luan<sup>1</sup>; <sup>1</sup>*Sun Yat-Sen University, Guangzhou, China*; <sup>2</sup>*China National Analytical Center Guangzhou, Guangzhou, China*; <sup>3</sup>*The Hong Kong Polytechnic University, Hong Kong SAR, China*
- TP 026 **Analysis of Butylene Glycol Oligomer Samples by Temperature-Rising Direct Analysis in Real Time Mass Spectrometry (TR-DART-MS);** Jun Watanabe<sup>1</sup>; Kazumasa Kinoshita<sup>2</sup>; Takao Nishiguchi<sup>2</sup>; Chikako Takei<sup>2</sup>; Motoshi Sakakura<sup>3</sup>; Teruhisa Shiota<sup>3</sup>; <sup>1</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>2</sup>*Bio Chromato, Inc., Fujisawa, Japan*; <sup>3</sup>*AMR, Inc., Tokyo, Japan*
- TP 027 **Development of a Simultaneous Analysis Method of Volatile Compounds by DART MS;** Takehito Sagawa<sup>1</sup>; Keiko Matsumoto<sup>2</sup>; Jun Watanabe<sup>2</sup>; Motoshi Sakakura<sup>3</sup>; Teruhisa Shiota<sup>3</sup>; <sup>1</sup>*S & B Foods Inc., Tokyo, Japan*; <sup>2</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>3</sup>*AMR, Inc., Tokyo, Japan*
- TP 028 **DART in Forensic Toxicology - Fast and Accurate Detection of Toxicants and Illicit Drugs in Human Blood and Urine Samples;** Ying Zhang<sup>1</sup>; Wei Zhang<sup>1</sup>; Wenfang Zhang<sup>1</sup>; Shiyang Qin<sup>1</sup>; Daming Zhang<sup>1</sup>; Xiaokun Duan<sup>2</sup>; Xiangtao Chen<sup>2</sup>; Charles C. Liu<sup>2</sup>; <sup>1</sup>*Beijing Public Security Bureau, Beijing, China*; <sup>2</sup>*ASPEC Technologies LTD, Beijing, China*

ION SPECTROSCOPY  
029-038

- TP 029 **Gas-Phase IRMPD Modeling of Deprotonated Peptide Binding Frameworks for Divalent Transition Metal Ions;** Robert C. Dunbar<sup>1</sup>; Jonathan Martens<sup>2</sup>; Giel Berden<sup>2</sup>; Jos Oomens<sup>2,3</sup>; <sup>1</sup>*Case Western Reserve Univ, Cleveland, OH*; <sup>2</sup>*Radboud University, Nijmegen, Netherlands*; <sup>3</sup>*University of Amsterdam, Amsterdam, Netherlands*
- TP 030 **Conformation-Specific IR-UV Double-Resonance Spectroscopy and Structural Analysis of Methyl Esterified Leucine Enkephalin;** Nicole Burke; Andrew DeBlase; James Redwine; John Hopkins; Timothy Zwier; Scott McLuckey; *Purdue University, Lafayette, IN*
- TP 031 **Proton Migration in Tryptophan-Containing Radicals Elucidated by Infrared Laser Spectroscopy;** Ning Zhao; *University of Florida, Gainesville, FL*
- TP 032 **Unimolecular Decomposition of M(Pro2-H)+ (M=Mg, Ca, Sr, Ba, Mn, Fe, Co, Ni, Cu, Zn) by IRMPD, SORI-CID, and Theoretical Studies;** Yasaman Jami Alahmadi; Travis D Fridgen; *Memorial University of NL, St. John's, Canada*
- TP 033 **Charge Solvation or Salt Bridge : Proton Affinity as a Structural Probe for Protonated Amino Acid Homodimers;** Xianglei Kong; *Nankai University, Tianjin, China*
- TP 034 **UltraViolet Action Spectroscopy of Peptidic Diazirines and Their Peptide Ion Complexes;** Robert Pepin<sup>1</sup>; Frantisek Turecek<sup>2</sup>; Steen Bronsted Nielsen<sup>3</sup>; <sup>1</sup>*U of Washington, Chemistry, Lakewood, WA*; <sup>2</sup>*University of Washington, Seattle, WA*; <sup>3</sup>*University of Aarhus, Aarhus, Denmark*



- TP 035 **Towards Probing Hydrogen Bonded Networks and Electron Transfer States through the Characterization of Fluorophores;** Vaishnavi Rajagopal; Alessandra Ferzoco; *Rowland Institute at Harvard, Cambridge, MA*
- TP 036 **Unravelling Environmental Effects on Light-Harvesters: Photodissociation Action Spectroscopy of Gas-Phase Chlorophylls and Porphyrins;** Sydney Wellman; Rebecca Jockusch; *Department of Chemistry, University of Toronto, Toronto, Canada*
- TP 037 **“Turn-On” Fluorophores to Probe the Conformation of Gaseous Biomolecules?** Martin Czar; Stephen Sciuto; Rebecca A. Jockusch; *Chemistry Department, University of Toronto, Toronto, Canada*
- TP 038 **Ultraviolet and Vacuum Ultraviolet Light Sources for Advanced Mass Spectrometry Techniques in Support of Nuclear Non-Proliferation;** David Willingham; Benjamin Naes; Mindy Zimmer; *Pacific Northwest National Laboratory, Richland, WA*
- ION/MOLECULE, ION/ION, ION/ELECTRON INTERACTIONS**  
039-060
- TP 039 **Strategies for Selective and Non-Selective Oxidative Labeling of Peptides and Proteins in the Gas-Phase via Ion/Ion Reactions;** Alice Pilo; Jiexun Bu; Scott McLuckey; *Purdue University, West Lafayette, IN*
- TP 040 **Roles of Metal-Peptide Interactions in Electron Capture Dissociation of Metal- $\beta$  Complexes;** Tao Jiang; Kristina Hakansson; *University of Michigan, Ann Arbor, MI*
- TP 041 **Gas-Phase Nucleophilic Substitution in Atmospheric Pressure Photoionization in the Presence of Halogenated Dopants;** Tiina J. Kauppila<sup>1</sup>; Hendrik Kersten<sup>2</sup>; Thorsten Benter<sup>2</sup>; <sup>1</sup>*University of Helsinki, Helsinki, Finland*; <sup>2</sup>*University of Wuppertal, Wuppertal, Germany*
- TP 042 **Multiply Charged Non-Covalent Complexes by UV/Vis-Photodissociation with Electron Transfer Dissociation and Collision-Induced Dissociation;** Andy Dang; Christopher Shaffer; Frantisek Turecek; *University of Washington, Seattle, WA*
- TP 043 **Design of Isoxazolium Reagents for the Gas-Phase Amidation of Carboxylic Acids via Ion/Ion Reactions;** Zhou Peng; Scott A. McLuckey; *Purdue University, West Lafayette, IN*
- TP 044 **Generation of Hydroxyalkyl Radicals with Photoinitiator and Their Reactions with CysteinyI Peptides;** Sarju Adhikari; Lei Tan; Yu Xia; *Purdue University, West Lafayette, IN*
- TP 045 **Alkali Metal Adduct Radical Cations of Cysteine Derivatives: A Gas-Phase Reactivity and Structural Elucidation Study;** Michael Lesslie<sup>1</sup>; Sandra Osburn<sup>2</sup>; Giel Berden<sup>3</sup>; Jos Oomens<sup>3</sup>; Michael J. Van Stipdonk<sup>4</sup>; Victor Ryzhov<sup>1</sup>; <sup>1</sup>*Northern Illinois University, Dekalb, IL*; <sup>2</sup>*Duquesne University, Munhall, PA*; <sup>3</sup>*Radboud University Nijmegen, Nijmegen, Netherlands*; <sup>4</sup>*Duquesne University, Pittsburgh, PA*
- TP 046 **Ion-Ion and Ion-Electron Activation Experiments in a Novel Linear Ion Trap;** Dimitris Papanastasiou<sup>1</sup>; Alexander Lekkas<sup>1</sup>; Diamantis Kounadis<sup>1</sup>; Ioannis Orfanopoulos<sup>1</sup>; Andreas Mpozatzidis<sup>1</sup>; Emmanouel Raptakis<sup>2</sup>; <sup>1</sup>*Fasmatech, Athens, Greece*; <sup>2</sup>*Fasmatech SA, Athens, Greece*
- TP 047 **Bending Gold(I) Dicoordinate Complexes to Switch on C-X  $\sigma$ -Bond Activation;** Athanasios Zavras<sup>1</sup>; Abderrahmane Amgoune<sup>2</sup>; Didier Bourissou<sup>2</sup>; Richard A. J. O’hair<sup>1</sup>; <sup>1</sup>*University of Melbourne, Victoria, Australia*; <sup>2</sup>*universite Paul Sabatier, Toulouse, France*
- TP 048 **Considerations for Attaining Improved ETD Performance for Top Down Applications;** Christopher Mullen; Lee Earley; Chad Weisbrod; John E. P. Syka; Jean-Jacques Dunyach; *Thermo Fisher Scientific, San Jose, CA*
- TP 049 **Conformational Differences of Leucine-Enkephalin Complexes Evaluated using Gas-Phase Hydrogen/Deuterium Exchange;** Yinjuan Chen<sup>1</sup>; Lei Yue<sup>2</sup>; Xunlei Ding<sup>3</sup>; Yuanjiang Pan<sup>2</sup>; Chuan-Fan Ding<sup>1</sup>; <sup>1</sup>*Fudan University, Shanghai, China*; <sup>2</sup>*Zhejiang University, Hangzhou, China*; <sup>3</sup>*North China Electric Power University, Beijing, China*
- TP 050 **Gas-Phase Ion/Molecule Reaction of CO<sub>2</sub> with Anilide Anions;** Chongming Liu; Athula B. Attygalle; *Stevens Institute of Technology, Hoboken, NJ*
- TP 051 **Gas-Phase Click Chemistry: 1,3-dipolar Cycloaddition of Alkynes with Azides via Ion/Ion Reactions;** Jiexun Bu; Scott McLuckey; *Purdue University, West Lafayette, IN*
- TP 052 **Impact of a Localized Radical Site on Dissociation of Peptides Modified Using an Alkyl-Nitroxide Spin Label Reagent;** Julia Aponte; Jennifer Brodbelt; *University of Texas Austin, Austin, TX*
- TP 053 **Identification of the Protonated Carboxylic Acid Functionality and Differentiation of Protonated Isomeric Hydroxybenzoic Acids via Regioselective Ion-Molecule Reactions;** Ravikiran Yerabolu<sup>1</sup>; John Kong<sup>1</sup>; Joann Max<sup>1</sup>; Raghavendhar Kotha<sup>1</sup>; Minli Zhang<sup>2</sup>; Hilka Kenttamaa<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, Indiana*; <sup>2</sup>*AstraZeneca, Boston, MA*
- TP 054 **Which Ion and Neutral Multipole and Anisotropic Polarizability Terms are Important in Ion—Molecule Collision Rates in Extreme Temperature Environments?** Kent M. Ervin; *University of Nevada, Reno, Reno, NV*
- TP 055 **Apparent Activation of H<sub>2</sub>O and Elimination of H<sub>2</sub> from Gas-Phase Mixed Metal Complexes;** Sandra Osburn; Alexandra Plaviak; Michael J. Van Stipdonk; *Duquesne University, Pittsburgh, PA*
- TP 056 **Integrated Ion Dynamics Simulations in OpenFOAM: Flow, Transport, Chemical Reactions and Space-Charge;** Walter Wissdorf; Thorsten Benter; *University of Wuppertal, Wuppertal, Germany*
- TP 057 **A Comparison of the Reactions of N-Methyl-6-dehydroquinolinium Cation with Nucleosides and Dinucleoside Phosphates in the Gas Phase and Aqueous Solution;** Joann Max; Ashley Wittrig; Fanny Widjaja; Hilka Kenttamaa; *Purdue University, West Lafayette, IN*
- TP 058 **Conformational Effects on the Proton Affinity of Lysine Homolog Containing Oligopeptides Studied by Mass Spectrometry and Infrared Multiphoton Dissociation Spectroscopy;** Patrickhenry Batoon; Jianhua Ren; *University of the Pacific, Stockton, CA*
- TP 059 **Probing Chemistry Using Molecular Beams and Vacuum Ultraviolet Synchrotron Radiation;** Biswajit Bandyopadhyay; Yigang Fang; Oleg Kostko; Musahid Ahmed; *Lawrence Berkeley National Laboratory, Berkeley, California*
- TP 060 **Identification of the N-Monosubstituted N-Hydroxylamino Functionality in Protonated Analytes via Ion/Molecule Reactions in Tandem Mass Spectrometry;** John Kong<sup>1</sup>; Huaming Sheng<sup>1</sup>; Weijuan Tang<sup>1</sup>; Ravikiran Yerabolu<sup>1</sup>; Peggy Williams<sup>1</sup>; Minli Zhang<sup>2</sup>; Hilka Kenttamaa<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*AstraZeneca, Boston, MA*
- INSTRUMENTATION: GENERAL**  
061-079
- TP 061 **PALMS: A Parallel Computational Engine for SIMION Simulating Multiple Ion Interactions;** Konstantin Novoselov; Vladimir M. Doroshenko; Alexander Misharin; *MassTech, Inc., Columbia, MD*
- TP 062 **Optimization of Ion Trap Isolation Methodology for Simultaneous Precursor Selection at the MS Level;** Philip M Remes<sup>1</sup>; Romain Huguet<sup>1</sup>; Jarrett Egertson<sup>2</sup>; Michael J. Maccoss<sup>2</sup>; Vlad Zabrouskov<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*Univ of Washington, Seattle, WA*

- TP 063 **Tracing Ions and Visualizing Charged Clusters in the Aerolens Under Transitory Gas Flow Conditions;** Emmanuel Raptakis<sup>1</sup>; Diamantis Kounadis<sup>1</sup>; Alexander Lekkas<sup>1</sup>; Athanasios Zacharos<sup>2</sup>; Ioannis Nikolos<sup>3</sup>; Dimitris Papanastasiou<sup>2</sup>; <sup>1</sup>Fasmatech SA, Athens, Greece; <sup>2</sup>Fasmatech, Athens, Greece; <sup>3</sup>Technical University of Crete, Chania, Greece
- TP 064 **Sub 500ps Magnetic Ion Detector with Extended Operating Life;** Dick Stresau; Yair Benari; Kevin Hunter; Peter Raffin; Wayne Sheils; Sid Sondur; Scott Morgan; *ETP Electron Multipliers, Clyde, Australia*
- TP 065 **Every Ion Counts: Optimization of the Quadrupole Mass Spectrometer for Improved Ion Transmission and Flat-Top Peaks;** Mariya J. Antony Joseph<sup>1</sup>; Simon Maher<sup>1,2</sup>; Fred P. M. Jjunju<sup>1</sup>; S. U. A. H. Syed<sup>3</sup>; John R. Gibson<sup>1</sup>; Iain S. Young<sup>2</sup>; Ron M. A. Heeren<sup>3</sup>; Stephen Taylor<sup>1</sup>; <sup>1</sup>Dept. of Electrical Engineering and Electronics, University of Liverpool, UK; <sup>2</sup>Institute of Integrative Biology, University of Liverpool, UK; <sup>3</sup>FOM Institute for Atomic and Molecular Physics, Amsterdam, Netherlands
- TP 066 **Improve Single Reaction Monitoring (SRM) Screening Speed by Using Parallel System Design on Mass Spectrometer Control System;** Qingyu Song; Eric Hemenway; Jew-Dong Kuo; Mary Blackburn; *Thermo Fisher Scientific, San Jose, CA*
- TP 067 **A New High-Resolution, Temperature-Variable Ion Mobility Mass Spectrometer;** Jakub Ujma<sup>1</sup>; Kevin Giles<sup>2</sup>; Michael Morris<sup>2</sup>; Perdita Barran<sup>1</sup>; <sup>1</sup>The University of Manchester, Manchester, UK; <sup>2</sup>Waters Corporation, Wilmslow, UK
- TP 068 **Next Generation Long Life Discrete-Dynode Detector;** Kevin Hunter; Russell Jurek; Dick Stresau; Scott Morgan; Wayne Sheils; *ETP Electron Multipliers, Clyde, Australia*
- TP 069 **Massively Parallel Simion Model of Quadrupole Analyzer Peak Shape;** Ken Newton; *Agilent Technologies, Santa Clara, CA*
- TP 070 **Enabling Fast Prototyping and Customization of Mass Spectrometer Control Software;** Jeff Brown; Emmy Hoyes; Richard Newton; Christopher Jones; Darren Hewitt; Wright Steven; Rennie Birch; David Langridge; Keith Richardson; Richard Chapman; *Waters Corporation, Wilmslow, UK*
- TP 071 **Simulation Results for Tolerance of Misalignment in Six Degrees of Freedom in Ceramic Plate Linear Ion Traps;** Qinghao Wu; Yuan Tian; Ailin Li; Daniel Austin; *Brigham Young University, Provo, UT*
- TP 072 **Fully Automated On-Line Sample Extraction and Analysis of Residual Pesticides in Agricultural Products by using On-Line SFE-SFC-MS;** Takanari Hattori<sup>1</sup>; Takato Uchikata<sup>1</sup>; Hidetoshi Terada<sup>1</sup>; Chigusa Ichikawa<sup>1</sup>; Yasuhiro Funada<sup>1</sup>; Yayoi Ichiki<sup>2</sup>; Miho Sakai<sup>3</sup>; Takashi Ando<sup>3</sup>; Yoshihiro Izumi<sup>4,5</sup>; Eiichiro Fukusaki<sup>5</sup>; Takeshi Bamba<sup>4,5</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>Miyazaki Enterprise Promotion Organization, Miyazaki, Japan; <sup>3</sup>Miyazaki Agricultural Research Institute, Miyazaki, Japan; <sup>4</sup>Kyushu University, Fukuoka, Japan; <sup>5</sup>Osaka University, Suita, Japan
- TP 073 **Surface Induced Dissociation Utilized to Characterize Protein Complexes Trapped in the Trap Cell of a Q-TOF Instrument;** Jing Yan<sup>1</sup>; Sophie R. Harvey<sup>1</sup>; Jeff Brown<sup>2</sup>; Emmy Hoyes<sup>2</sup>; Vicki H. Wysocki<sup>1</sup>; <sup>1</sup>The Ohio State University, Columbus, OH; <sup>2</sup>Waters Corporation, Wilmslow, UK
- TP 074 **Ion Mobility-Selected Trapping and Enrichment in Structures for Lossless Ion Manipulations (SLIM);** Tsung-Chi Chen; Jeremy A. Sandoval; Spencer A. Prost; William E. Karnesky; Xing Zhang; Ian K. Webb; Ahmed M. Hamid; Randolph V. Norheim; Erin S. Baker; Yehia M. Ibrahim; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- TP 075 **Velocity Distribution Measurement of Fullerene Ions with and without Quadrupole Fields;** Avinash Patil; Sin-Ciang Jiang; Kai-Chun Yen; Szu-Wei Chou; Wen-Ping Peng; *National Dong Hwa University, Shoufeng, Hualien, Taiwan*
- TP 076 **Enhancing Ion Sampling Efficiency, Ion Transmission and Detection on a Triple Quadrupole Platform;** Natsuyo Asano; Manabu Ueda; Wataru Fukui; Tairo Ogura; Kazuo Mukaibatake; *Shimadzu Corporation, Kyoto, Japan*
- TP 077 **Quantifying and Improving the Lifetime of Hybrid Detectors;** Stephen Ritzau; Matthew Breuer; Bruce Laprade; Jason Alston; *PHOTONIS USA, Sturbridge, MA*
- TP 078 **High-Throughput Serum Peptide Profiling of a Clinical Cancer Cohort on a Novel MALDI-TOF-MS Platform;** Yuri E.M. Van Der Burgt<sup>2</sup>; Hans Dalebout<sup>2</sup>; Simone Nicolardi<sup>2</sup>; Marco R. Bladergroen<sup>2</sup>; Wilma E. Mesker<sup>1</sup>; Rob A.E.M. Tollenaar<sup>1</sup>; Magnus Palmblad<sup>2</sup>; <sup>1</sup>Leiden University Medical Center, Leiden, Netherlands; <sup>2</sup>Center for Proteomics and Metabolomics, LUMC, Leiden, Netherlands
- TP 079 **Trajectory Calculations of Space Charge Effects in Ion Traps via an Iterative Solution of the Poisson Equation;** David Langridge; *Waters, Wilmslow, UK*
- INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION AND SAMPLING**  
080-099
- TP 080 **Characterizing an ESI-MS Interface Based on the Ion Utilization Efficiency;** Jonathan Cox<sup>1</sup>; Ioan Marginean<sup>2</sup>; Richard Smith<sup>1</sup>; Keqi Tang<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>GWU, Washington, DC
- TP 081 **The Correlations between Ions and Neutrals in Matrix-Assisted Laser Desorption/Ionization;** I-Chung Lu; Yuan Tseh Lee; Chi-Kung Ni; *Institute of Atomic and Molecular Sciences, Academ, Taipei, Taiwan*
- TP 082 **Aerodynamic Focusing Extractive Electrospray Ionization;** Bijay Banstola; Fabrizio Donnarumma; Kermit K. Murray; *Louisiana State University, Baton Rouge, LA*
- TP 083 **Soft Ionization, NIST identification and Capabilities for Quantitative Analysis in Conditioned Glow Discharge Ion Source;** Alexander Kolosov; Anatoly Verenchikov; *MSC-CG, Bar, Montenegro*
- TP 084 **Development of a Paper Spray Cartridge with Integrated SPE to Improve Sensitivity for Drug Detection;** Chengsen Zhang; Nicholas Manicke<sup>\*</sup>; *IUPUI, Indianapolis, IN*
- TP 085 **Thermal Analysis-Photo Ionization Mass Spectrometry (TA-PIMS) for Analysis of Crude Oils and Toxic Tricresylphosphates in Jet-Turbine Oils;** Mohammad Reza Saraji-Bozorgzad<sup>1</sup>; Thorsten Streibel<sup>2</sup>; Robert Geissler<sup>3</sup>; Andreas Walte<sup>4</sup>; Thomas Denner<sup>5</sup>; Ralf Zimmermann<sup>6</sup>; <sup>1</sup>Photonion GmbH, Neuherberg, Germany; <sup>2</sup>University Rostock, Rostock, Germany; <sup>3</sup>Helmholtz Zentrum München, Munich, Germany; <sup>4</sup>Photonion GmbH, Schwerin, Germany; <sup>5</sup>Netzsch Gerätebau GmbH, Selb, Germany; <sup>6</sup>University of Rostock, Rostock, N/A
- TP 086 **Catalytic Effects of Electro sprayed Molecular Ions;** Abraham Badu Tawiah; *Ohio State University, Columbus, OH*
- TP 087 **Methodologies for Reducing the Charge of Electrospray Generated Ions;** Liang Wang; Peter T A Reilly; *Washington State University, Pullman, WA*
- TP 088 **Development of a High-Flux Ion Soft-Landing Instrument for Preparation of Cluster-Based Supercapacitor Devices;** Venkateshkumar Prabhakaran; Don Gunaratne; Yehia Ibrahim; Randolph Norheim; Grant Johnson; Julia Laskin; *Pacific Northwest National Laboratory, Richland, WA*
- TP 089 **Suppressing the Background Interference and Enhancing the Performance of Electrospray Ionization Mass Spectrometry by Doping Concentrated Gaseous Acetonitrile;** Fangjun Wang; Hanfa Zou; *Dalian, China*





- TP 090 **Multiplexed Tandem Mass Spectrometry by Modulation of Ionization Efficiency;** Sepideh Rahbarirad; Andre Venter; *Western Michigan University, Kalamazoo, MI*
- TP 091 **A Demonstration of the Organic Detection Capabilities of a Two Step Laser Desorption/Ionization Time-of-Flight Mass Spectrometer;** Kyle Uckert<sup>1</sup>; Stephanie Getty<sup>2</sup>; Andrej Grubisic<sup>3</sup>; Xiang Li<sup>4</sup>; William Brinckerhoff<sup>2</sup>; Timothy Cornish<sup>5</sup>; Nancy Chanover<sup>1</sup>; Jamie E. Elsil<sup>2</sup>; Richard Zare<sup>6</sup>; <sup>1</sup>New Mexico State University, Las Cruces, NM; <sup>2</sup>NASA GSFC, Greenbelt, MD; <sup>3</sup>University of Maryland, College Park, MD; <sup>4</sup>University of Maryland, Baltimore County, Greenbelt, MD; <sup>5</sup>C&E Research, Inc., Columbia, MD; <sup>6</sup>Stanford University, Stanford, Ca
- TP 092 **A Universal Source for Ionization of Polar and Nonpolar Compounds: Testing Its Applicability to Petroleomic Studies;** Heliara Lopes Nascimento<sup>1</sup>; Marcos Pudenz<sup>1</sup>; Vanessa Santos<sup>1</sup>; Celio Fernando Angolini<sup>1</sup>; Pedro Vendramini<sup>1</sup>; Jose Luiz Jara<sup>1</sup>; Rosana Cardoso Lopes Pereira<sup>2</sup>; Wagner Leonel Bastos<sup>2</sup>; Michael Murgu<sup>3</sup>; Marcos N. Eberlin<sup>1</sup>; <sup>1</sup>thomson Unicamp- Brazil, Sao Paulo, Brazil; <sup>2</sup>Petrobras, RJ, Brazil; <sup>3</sup>Waters Brazil, Barueri, SP - Brazil
- TP 093 **Selective Ionization of Carboxylic Acids for Positive Ion Tandem Mass Spectrometric Analyses in Complex Environmental and Bioanalytical Samples;** Kyle D. Duncan<sup>1,2</sup>; Erik T. Krogh<sup>1,2</sup>; Christopher G. Gill<sup>1,2</sup>; <sup>1</sup>University of Victoria, Victoria, BC, Canada; <sup>2</sup>Appl. Env. Res. Labs. (AERL), Nanaimo, BC, Canada
- TP 094 **Understanding the Relationship of Silicon Surface Morphologies and their Nanostructure-Initiator Mass Spectrometry (NIMS) Sensitivity;** Jian Gao; Markus De Raad; Ron Zuckermann; Trent Northen; *Lawrence Berkeley National Lab, Berkeley, CA*
- TP 095 **The PhoTorrent™ Atmospheric Pressure Photoionization (APPI) Source Utilized for High Efficiency Photoionization of Testosterone and 25-OH Vitamin D3;** Ellie Majdi; Frenny Ruparella; Sha Joshua Ye; *IONICS Mass Spectrometry, Bolton, Canada*
- TP 096 **Enhancing Ion Abundances of Oligosaccharides by the Marangoni Effect in MALDI Mass spectrometry;** Yin-Hung Lai; Yi-Hong Cai; Yi-Sheng Wang; *Genomics Research Center, Taipei, Taiwan*
- TP 097 **The Use of Bursting Bubbles for the Specific Enrichment and Direct Molecular Analysis of Chemicals in Bulk Solution;** Yunfeng Cai; Konstantin Chingjin; Juchao Liang; Eric Handberg; Huanwen Chen; *East China Institute of Tech., Nanchang, China*
- TP 098 **Signal Decrease and Recovery in MALDI and Guidelines for Choosing New Matrices;** Chih-Yuan Lin<sup>1</sup>; I-Chung Lu<sup>2</sup>; Jien Lian Chen<sup>1</sup>; Hou-Yu Lin<sup>1</sup>; Yuan Tseh Lee<sup>1</sup>; Chi-Kung Nj<sup>1</sup>; <sup>1</sup>Institute of Atomic and Molecular Sciences, Academ, Taipei, Taiwan; <sup>2</sup>academia Sinica, Taipei, Taiwan
- TP 099 **Laser Desorption-Radio Frequency Ionization (LD-RFI);** Matthew R. Brantley; Abayomi D. Olaitan; Touradj Solouki; *Department of Chemistry and Biochemistry, Baylor University, Waco, TX*
- HIGH MAS ACCURACY/HIGH PERFORMANCE MS: APPLICATIONS**  
100-117
- TP 100 **Characterization of Dissolved Organic Matter from Brazilian Marine and Fresh Water by High Resolution Mass Spectrometry;** Jose Javier Melendez; Marcos Eberlin; *Campinas, Brazil*
- TP 101 **Pharmaceutical Impurity Profiling on a Novel Q-TOF Platform with Particle SWARM Optimization Technology and Optimized Beam Shaping Optics;** Christian Klein<sup>1</sup>; Dorothy Yang<sup>1</sup>; Ken Imatani<sup>1</sup>; Pat Sandra<sup>2</sup>; Koen Sandra<sup>2</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>RIC, Kortrijk, Belgium
- TP 102 **Development of Un-targeted Screening Method for Detection of Synthetic PDE-5 Inhibitor Drugs and Analogues Adulterated in Health Supplements on LCMS-IT-TOF;** Jie Xing<sup>1</sup>; Dinash Aravind<sup>2</sup>; Zhe Sun<sup>1</sup>; May Yen Ang<sup>3</sup>; Zhaoqi Zhan<sup>1</sup>; <sup>1</sup>Shimadzu (Asia Pacific) Pte Ltd, 79 Science Park, Drive #02-01/08, Singapore 118264; <sup>2</sup>National Pharmaceutical Control Bureau, Jalan, Universiti, 46200 Petaling Jaya, Selangor, Malaysia; <sup>3</sup>Shimadzu Malaysia Sdn Bhd, Kota Damansara,, 47810 Petaling Jaya, Selangor, Malaysia
- TP 103 **Comprehensive Characterization of Low Molecular Weight Heparins Using High Resolution Mass Spectrometry;** Annu Uppal; Dipankar Malakar; Faraz Rashid; Manoj Pillai; *SCIEX, 121, Udyog Vihar, Phase IV, Gurgaon, Haryana, India*
- TP 104 **Forensic Analysis of Brand and Imitation Perfume Samples with GC, GC×GC, and HR-TOFMS;** Elizabeth Humston-Fulmer; Michelle Page; Joe Binkley; *LECO Corporation, St. Joseph, MI*
- TP 105 **Specific LC-High-Resolution-MS Guidelines for the Validation of Quantitative Methods and Intraday Assays;** Baptiste Grund<sup>1</sup>; Hugues Henry<sup>1</sup>; Maciej Bromirski<sup>2</sup>; Bertrand Rochat<sup>1</sup>; <sup>1</sup>CHUV, Lausanne, Switzerland; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany
- TP 106 **Characterization of humic acid from Brazilian soils by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Monica Johanna Martinez Mejia; Susanne Rath; Marcos Nogueira Eberlin; *UNICAMP, Campinas, Brazil*
- TP 107 **Structural Characterization of MS/MS Product Ions Selected for the Detection of Regulated Veterinary Drugs;** Alberto Nuñez; Steven Lehotay; *USDA-ARS-ERRC, Wyndmoor, PA*
- TP 108 **A High Resolution Accurate Mass Approach for the Quantitation of Buprenorphine and Paroxetine in Rat Plasma;** Keeley Murphy<sup>1</sup>; Jonathan L. Josephs<sup>2</sup>; Maciej Bromirski<sup>3</sup>; Olaf Scheibner<sup>4</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Scientific, West Windsor, NJ; <sup>3</sup>Thermo Fisher Scientific GmbH, Bremen, N/A; <sup>4</sup>Thermo Fisher Scientific, Bremen, Germany
- TP 109 **Enhancing Precursor and Product Ion Alignment of Chimeric Spectra;** Roy Martin; Steve Ciavarini; Brad Williams; Scott Geromanos; *Waters Corporation, Milford, MA*
- TP 110 **Core Facility Workflow for Characterization of Intact Proteins via High Resolution Mass Spectrometry;** Andre Bui; John O'brien; Maria Person; *University of Texas, Austin, TX*
- TP 111 **Interpretation of Two-Dimensional FT-ICR Mass Spectra: Noise, Phase and Isotopes;** Maria van Agthoven<sup>1</sup>; Mark Barrow<sup>1</sup>; Lionel Chiron<sup>2</sup>; Marie-Aude Coutouly<sup>4</sup>; Christopher Wootton<sup>1</sup>; Federico Floris<sup>1</sup>; Marc-André Delsuc<sup>3</sup>; Christian Rolando<sup>5</sup>; Peter B. O'connor<sup>1</sup>; <sup>1</sup>University of Warwick, Coventry, UK; <sup>2</sup>CASC4DE, Illkirch-Graffenstaden, France; <sup>3</sup>IGBMC, Illkirch-Graffenstaden, France; <sup>4</sup>NMRTEC, Illkirch-Graffenstaden, France; <sup>5</sup>Université Lille 1, Sciences et Technologies, Villeneuve d'Ascq, France
- TP 112 **Improved Characterization of Complex Proteins using Middle-Down 193 nm Ultraviolet Photodissociation;** Victoria C. Cotham; Jennifer S. Brodbelt; *University of Texas at Austin, Austin, TX*
- TP 113 **Sensitive Negative Chemical Ionization, Accurate Mass as Resolution and Detection Power—a New Approach to Analysis of Chlorinated Paraffins by GC/Q-TOF;** Wei Gao<sup>1</sup>; Yawei Wang<sup>1</sup>; Wenwen Wang<sup>2</sup>; <sup>1</sup>Research Center for Eco-Environmental Sciences, Beijing, China; <sup>2</sup>Agilent Technologies, Beijing, China

- TP 114 **A Streamlined Workflow for the Profiling of Impurities Using High Resolution Accurate Mass Spectrometry;** Jason Causon; *AB SCIEX, Warrington, UK*
- TP 115 **Exploring the Complexity of Yeast Using Enhanced Chromatographic/Mass Spectral Resolution;** David Alonso; Jeff Patrick; Joe Binkley; *Leco Corporation, St. Joseph, MI*
- TP 116 **Peptide de novo Sequencing via Paired Single Residue-Transposed Digestions and Ultrahigh Resolution Fourier Transform Ion Cyclotron Resonance Tandem Mass Spectrometry;** Naomi Brownstein<sup>1,2</sup>; Xiaoyan Guan<sup>1</sup>; Yuan Mao<sup>3</sup>; Qian Zhang<sup>2</sup>; Peter DiMaggio<sup>4</sup>; Qiangwei Xia<sup>2,3</sup>; Lichao Zhang<sup>5</sup>; Alan Marshall<sup>6</sup>; Nicolas L. Young<sup>7</sup>; <sup>1</sup>National High Magnetic Field Lab, Tallahassee, FL; <sup>2</sup>Florida State University, Tallahassee, Florida; <sup>3</sup>Regeneron Pharmaceuticals, Inc., Tarrytown, NY; <sup>4</sup>Imperial College London, South Kensington Campus, London, UK; <sup>5</sup>University of Virginia, Charlottesville, VA; <sup>6</sup>Ion Cyclotron Resonance Prog, Tallahassee, FL; <sup>7</sup>NHMFL / FSU, Tallahassee, FL
- TP 117 **Low-Abundance Isotope Enrichment in Individual Muscle Proteins Measured by High-Resolution Mass Spectrometry;** Kelly Hines<sup>1,2</sup>; G. Charles Ford<sup>1</sup>; Katherine Klaus<sup>2</sup>; Brian Irving<sup>2</sup>; Beverly Ford<sup>1</sup>; Kenneth Johnson<sup>3</sup>; Ian Lanza<sup>1,2</sup>; K. Sreekumaran Nair<sup>1,2</sup>; <sup>1</sup>Mayo Clinic Metabolomics Resource Core, Rochester, MN; <sup>2</sup>Mayo Clinic Division of Endocrinology, Rochester, MN; <sup>3</sup>Mayo Clinic Medical Genome Facility Proteomic Core, Rochester, MN

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- TP 119 **Investigation of Self-Calibrated, Fine-Isotope-Line Fit Scoring in Combined HPLC-Fourier Transform Orbital Trapping MS for Candidate Formulae Elimination;** Yongdong Wang; Ming Gu; *Cerno Bioscience, Norwalk, CT*
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- TP 121 **Dynamic Range Extension in FT-ICR Mass Spectrometry by Spectral Segmentation;** Logan C. Krajewski<sup>1</sup>; Christopher L. Hendrickson<sup>1,2</sup>; Christie G. Enke<sup>3</sup>; Alan G. Marshall<sup>1,2</sup>; <sup>1</sup>Department of Chemistry and Biochemistry, FSU, Tallahassee, FL; <sup>2</sup>National High Magnetic Field Laboratory, FSU, Tallahassee, FL; <sup>3</sup>University of New Mexico, Placitas, NM
- TP 122 **Absorption Mode Gets Even Better with its Svelte New Curves;** David Kilgour<sup>1</sup>; Konstantin Nagornov<sup>2</sup>; Steven Van Orden<sup>3</sup>; Anton Kozhinov<sup>2</sup>; Konstantin Zhurov<sup>2</sup>; Yury Tsybin<sup>2,4</sup>; David Goodlett<sup>1</sup>; <sup>1</sup>University of Maryland Baltimore, Baltimore, MD; <sup>2</sup>Ecole Polytechnique Fédérale, Lausanne, Switzerland; <sup>3</sup>Bruker Daltonics Inc., Billerica, MA; <sup>4</sup>Spectroswiss Sàrl, Lausanne, Switzerland
- TP 123 **A Novel Method of m/z Drift Correction for oa-TOF Mass Spectrometers based on Construction of Libraries of 'Matrix' Components;** Martin Green; Keith Richardson; Martin Palmer; Nick Tomczyk; *Waters Corporation, Manchester, UK*
- TP 124 **Improvements for High-Resolution Analysis on a Modified Tribrid Mass Spectrometer;** Jesse D. Canterbury<sup>1</sup>; Nick Izgarian<sup>1</sup>; Michael W. Senko<sup>1</sup>; Eduard Denisov<sup>2</sup>; Alexander Makarov<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- TP 125 **Generation of Absorption-Mode FT Mass Spectra from a Commercial Data Station;** Greg T. Blakney<sup>1</sup>; Donald F. Smith<sup>1</sup>; Nathan K. Kaiser<sup>1</sup>; Steven C. Beu<sup>2</sup>; Alan Marshall<sup>1,3</sup>; Christopher L. Hendrickson<sup>1</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>S C Beu Consulting, Austin, TX; <sup>3</sup>Dept of Chemistry/Biochemistry, Florida State Univ, Tallahassee, FL
- TP 126 **Frequency Multiplication for High-Throughput Fourier-Transform Ion Cyclotron Resonance Mass Spectrometry;** Tzu-Yung Lin<sup>1</sup>; Mikhail V. Gorshkov<sup>2</sup>; Aleksey V. Tolmachev<sup>1</sup>; Jared B. Shaw<sup>1</sup>; Rosalie K. Chu<sup>1</sup>; Richard Harkewicz<sup>1</sup>; R. James Ewing<sup>1</sup>; Mowei Zhou<sup>1</sup>; David W. Koppenaal<sup>1</sup>; Errol W. Robinson<sup>1</sup>; Ljiljana Pasa-Tolic<sup>1</sup>; <sup>1</sup>Pacific Northwest National Lab, Richland, WA; <sup>2</sup>INEPCP RAS, Moscow, Russian Federation

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- TP 129 **A Pipeline for Integration and Visualization of Breast Cancer Subtype-Specific Peptidome;** John A. Wrobel<sup>1</sup>; Harsha P. Gunawardena<sup>1</sup>; Jonathon O'Brien<sup>1</sup>; Ling Xie<sup>1</sup>; Kelly Ruggles<sup>2</sup>; David Fenyo<sup>2</sup>; Sherri Davies<sup>3</sup>; Bhajat Qaqish<sup>1</sup>; Ding Li<sup>3</sup>; Reid Townsend<sup>3</sup>; Matthew Ellis<sup>3</sup>; Xian Chen<sup>1</sup>; <sup>1</sup>University of North Carolina at Chapel Hill, Chapel Hill, NC; <sup>2</sup>NYU Langone Medical Center, New York, NY; <sup>3</sup>Washington University School of Medicine, St. Louis, MO
- TP 130 **BatMass: Developer Friendly Extensible Software Platform for Visualization and Analysis of Raw MS Data and Processed Results;** Dmitry Avtonomov; Chih-Chiang Tsou; Alexander Raskind; Alexey Nesvizhskii; *University of Michigan, Ann Arbor, MI*
- TP 131 **Plugging Proteomics Peptide-Spectral Match Visualization into Galaxy;** James Johnson<sup>1</sup>; Thomas McGowan<sup>1</sup>; Ira Cooke<sup>2</sup>; John Chilton<sup>3</sup>; Pratik Jagtap<sup>4</sup>; Timothy J. Griffin<sup>1</sup>; <sup>1</sup>University of Minnesota, Minneapolis, MN; <sup>2</sup>La Trobe University, Melbourne, Australia; <sup>3</sup>Penn State University, State College, PA; <sup>4</sup>Center for Mass Spectrometry and Proteomics, UMN, St. Paul, MN
- TP 132 **Panorama Public: A Public Repository for Skyline Documents;** Vagisha Sharma<sup>1</sup>; Josh Eckels<sup>2</sup>; Birgit Schilling<sup>3</sup>; Jacob D. Jaffe<sup>4</sup>; Michael J. Maccoss<sup>1</sup>; Brendan Maclean<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>LabKey Software, Seattle, WA; <sup>3</sup>Buck Institute for Research on Aging, Novato, CA; <sup>4</sup>The Broad Institute, Cambridge, MA
- TP 133 **Mass Spectrometry Quality Control: Instrument Monitoring and Pattern Mining Insights;** Wout Bittremieux<sup>1</sup>; Hanny Willems<sup>2</sup>; Lennart Martens<sup>3</sup>; Dirk Valkenburg<sup>2</sup>; Kris Laukens<sup>1</sup>; <sup>1</sup>University of Antwerp, Antwerp, Belgium; <sup>2</sup>VITO, Mol, Belgium; <sup>3</sup>University of Ghent, Ghent, Belgium



- TP 134 **Performing Quality Control on Targeted Proteomics Assays using Skyline and Panorama**; Josh Eckels<sup>1</sup>; Vagisha Sharma<sup>3</sup>; Yuval Boss<sup>3</sup>; Huilin Shi<sup>3</sup>; Tom Dunkley<sup>4</sup>; Kristin Wildsmith<sup>5</sup>; Cory Nathe<sup>2</sup>; Aaron Robinson<sup>2</sup>; Richard S. Johnson<sup>6</sup>; Jacob D. Jaffe<sup>7</sup>; Michael J. Maccoss<sup>3</sup>; Brendan Maclean<sup>3</sup>; <sup>1</sup>LabKey Software, San Diego, CA; <sup>2</sup>LabKey Software, Seattle, WA; <sup>3</sup>University of Washington, Seattle, WA; <sup>4</sup>F. Hoffmann-La Roche Ltd, Basel, Switzerland; <sup>5</sup>Genentech, Inc, San Francisco, CA; <sup>6</sup>University of Washington, Mercer Island, WA; <sup>7</sup>The Broad Institute, Cambridge, MA
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- TP 144 **SWATH Profiling of MAPK Pathway Mutant Cancer Cell Lines Reveals Similarities in response to drug inhibition independent of cell type**; Christoph Krisp; Matthew McKay; Mark Molloy; *Australian Proteome Analysis Facility, Sydney, Australia*
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- TP 154 **Targeted Determination of Site-Specific N-Glycosylation on B Cell Antigen Receptor Using Data-Independent Acquisition**; Kuan-Ting Pan<sup>1</sup>; Chen-Chun Chen<sup>2</sup>; Kay-Hooi Khoo<sup>3</sup>; Henning Urlaub<sup>1,4</sup>; <sup>1</sup>Bioanal. MS Group, Max Plank Inst for Biophys Chem, Goettingen, Germany; <sup>2</sup>Genomics

- Research Center, Academia Sinica, Taipei, Taiwan; <sup>3</sup>Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan; <sup>4</sup>Dept. of Clin. Chem., Univ. Med. Center Goettingen, Goettingen, Germany
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- TP 161 **Data-Dependent and Data-Independent Quantitative Analysis Applied in Parallel to the Study of Human Hippocampal Synaptosomes in Alzheimer's Disease**; Cheryl F. Lichti<sup>1</sup>; Wen-Ru Zhang<sup>1</sup>; Petra Erdmann-Gillmore<sup>2</sup>; Rose Connors<sup>2</sup>; Yiling Mi<sup>2</sup>; Jason M. Held<sup>2</sup>; Giulio Tagliatela<sup>1</sup>; <sup>1</sup>*Univ. of TX Medical Branch, Galveston, TX*; <sup>2</sup>*Washington University, Saint Louis, MO*
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- TP 163 **Bottom-Up Peptide Analysis by Stable Isotope Ion Mobility Data-Independent Acquisition Proteomics**; Jaimoen Majmudar; James Lawniczak; Ashesh Prakash; Brent Martin; *University of Michigan, Ann Arbor, MI*
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- TP 172 **Feasibility of Early Detection of Acute Pulmonary Exacerbations by Exhaled Breath Condensate Metabolomics**; Xiaoling Zang<sup>1</sup>; María Monge<sup>1,3</sup>; Nael McCarty<sup>2</sup>; Arlene Stecenko<sup>2</sup>; Facundo Fernández<sup>1</sup>; <sup>1</sup>*Georgia Institute of Technology, Atlanta, GA*; <sup>2</sup>*Emory University, Atlanta, GA*; <sup>3</sup>*National Scientific and Technical Research Council, Buenos Aires, Argentina*
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- TP 174 **Global Metabolite Profiling Study in Rat Heart Tissues Associated with Myocardial Infarction**; Miso Nam<sup>1,2</sup>; Youngae Jung<sup>1</sup>; Jueun Lee<sup>1</sup>; Do Hyun Ryu<sup>2</sup>; Geum-Sook Hwang<sup>1,3</sup>; <sup>1</sup>*KBSI, Seoul, Korea*; <sup>2</sup>*sungkyunkwan University, Suwon, Korea*; <sup>3</sup>*GRAS, Daejeon, Korea*
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- TP 176 **Parameter Optimization for Data Dependent Acquisitions in Metabolomics on an Orbitrap Fusion Tribrid Mass Spectrometer**; Ulli Hohenester<sup>1</sup>; Pierre Barbier Saint Hilaire<sup>1</sup>; Benoit Colsch<sup>1</sup>; Francois Fenaille<sup>1</sup>; Marie-Françoise Olivier<sup>1</sup>; Richard B. Cole<sup>2</sup>; Jean-Claude Tabet<sup>1</sup>; Christophe Junot<sup>1</sup>; <sup>1</sup>*CEA de Saclay, Gif sur Yvette Cedex, France*; <sup>2</sup>*Univ. P. et M. Curie (Paris 6), Paris Cedex 05, France*
- TP 177 **Metabolic Profiling of Human Pluripotent Stem Cell Derived Endothelial Cells**; Andreas A. Staempfli<sup>1</sup>; Christoph Patsch<sup>1</sup>; Gregor Dernick<sup>1</sup>; Martin Graf<sup>1</sup>; Stephan Mueller<sup>1</sup>; Michael Hennig<sup>1</sup>; Natalie Bordag<sup>2</sup>; <sup>1</sup>*F. Hoffmann-La Roche AG, Basel, Switzerland*; <sup>2</sup>*metanomics GmbH, Berlin, Germany*
- TP 178 **Complete Annotation of the Untargeted, LC/MS-Based Metabolomic Analysis of *Escherichia coli***; Nathaniel Mahieu; Amanda Chen; Xiaojing Huang; Gary J. Patti; *Washington University, St. Louis, MO*

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- TP 164 **Cortex Metabolome Response to Chronic Arsenic Exposure via Drinking Water**; Chensong Pan<sup>1</sup>; Jie Zhang<sup>2</sup>; Sawyen Ow<sup>3</sup>; Bingjie Liu<sup>1</sup>; <sup>1</sup>*Bruker (Beijing) Scientific Technology Co. Ltd., Beijing, China*; <sup>2</sup>*Institute of Urban Environment, CAS, Xiamen, China*; <sup>3</sup>*Bruker Daltonics Pte Ltd., Singapore, Singapore*
- TP 165 **Mapping Multiple Nutrient Fates Simultaneously with Metabolomics Using the Q-Exactive Orbitrap**; Liz Payne; Kevin Cho; Xiaojing Huang; Gary J. Patti; *Washington University School of Medicine, St. Louis, MO*



- TP 179 **Rapid Differential Expression Analysis of the Interactions of Metabolites Genotype-Pathogens in cacao (*Theobroma cacao* L.) Genotypes Infected by *Ceratomyces cacaoifunesta***; Fábio Santos<sup>1</sup>; Dilze Magalhães<sup>2</sup>; Edna Luz<sup>2</sup>; Marcos Eberlin<sup>1</sup>; <sup>1</sup>UNICAMP, Campinas, Brazil; <sup>2</sup>CEPLAC, Ilhéus, Bahia, Brazil
- TP 180 **Elucidation of Biochemical Basis of Scab Resistance in Pecan Using Metabolomics**; Zhentian Lei; Shelagh Henson; David Huhman; Bonnie Watson; Lloyd Sumner; The Samuel Roberts Noble Foundation, Ardmore, OK
- TP 181 **Development of High-Performance Chemical Isotope Labeling LC-MS for Parallel Metabolomic Profiling of Cerebrospinal Fluid and Serum in Spinal Cord Injury**; Yiman Wu<sup>1</sup>; Femke Streijger<sup>2</sup>; Brian K. Kwon<sup>2,3</sup>; Liang Li<sup>1</sup>; <sup>1</sup>Dept. of Chemistry, University of Alberta, Edmonton, Canada; <sup>2</sup>ICORD, University of British Columbia, Vancouver, Canada; <sup>3</sup>Dept. of Orthopaedics, Vancouver Spine Surgery Inst, Vancouver, Canada
- TP 182 **Metabolite Profiling and Geological Fingerprinting of Angelica Radix by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry**; Eunjung Son<sup>1,3</sup>; Min-Sun Kim<sup>1</sup>; A-Young Lee<sup>2</sup>; Dong-Seon Kim<sup>2</sup>; Mee Ree Kim<sup>3</sup>; Hyun Sik Kim<sup>1</sup>; <sup>1</sup>KBKI, Cheongju-Si, S. KOREA; <sup>2</sup>KIOM, Dajeon, Youseong-Ku; <sup>3</sup>CNU, Dajeon, Youseong-Ku
- TP 183 **Differentiating Yeast Strains by Untargeted Metabolomics Using UHPLC-HRMS/MS**; Biao Ji<sup>1</sup>; Joanie Emond<sup>1</sup>; Jennifer Chiang<sup>2</sup>; Guri Giaever<sup>2</sup>; Corey Nislow<sup>2</sup>; Lekha Sleno<sup>1</sup>; <sup>1</sup>UQAM, Montreal, Canada; <sup>2</sup>UBC, Vancouver, Canada
- TP 184 **Towards Comprehensive Coverage of the Zebrafish Embryo Metabolome using Liquid Chromatography Time of Flight Mass Spectrometry (LC-TOF-MS)**; Jeremiah Kelley; Claudia Maier; Oregon State University, Department of Chemistry, Corvallis, OR
- TP 185 **Elucidating New Pathways in Cancer Metabolism by Untargeted Metabolomic Profiling of Isotopic Fates**; Ying-Jr Amanda Chen<sup>1</sup>; Xiaojing Huang<sup>2</sup>; Nathaniel Mahieu<sup>1</sup>; Kevin Cho<sup>2</sup>; Gary J. Patti<sup>1,2</sup>; <sup>1</sup>Washington University, St Louis, MO; <sup>2</sup>Washington University School of Medicine, St. Louis, MO
- TP 186 **GC/MS Metabolomic Analysis for the Optimization of Chondrocyte Differentiation of Mesenchymal Stem Cells in 3D Pellet Culture**; Shujuan Tao; Andrea R. Tan; David Chen; Lewis M. Brown; Clark T. Hung; Columbia University, New York, NY
- TP 187 **Structural Elucidation of the Metabolome using Isotopic Ratio Outlier Analysis (IROA) in combination with UHPLC-QTOF and Data-Independent Acquisition**; Chris Beecher<sup>1</sup>; Felice de Jong<sup>1</sup>; Giuseppe Astarita<sup>2</sup>; <sup>1</sup>IROA Technologies, Ann Arbor, MI; <sup>2</sup>Waters Corporation, Milford, MA
- TP 188 **Untargeted Metabolomic Analysis of the Yeast Lipin Phosphatidate Phosphatase (Pah1p) Deletion Using Isotopic Ratio Outlier Analysis (IROA) and LC-HRMS**; Yu-Hsuan Tsai<sup>1</sup>; Timothy Garrett<sup>2</sup>; Yunping Qiu<sup>3</sup>; Robyn Moir<sup>4</sup>; Ian Willis<sup>4</sup>; Chris Beecher<sup>2</sup>; Richard Yost<sup>1,2</sup>; Irwin Kurland<sup>3</sup>; <sup>1</sup>Dept. of Chemistry, Univ. of Florida, Gainesville, FL; <sup>2</sup>Dept. of Pathology, Univ. of Florida, Gainesville, FL; <sup>3</sup>Dept. of Medicine, Albert Einstein College of, Bronx, NY; <sup>4</sup>Dept. of Biochemistry, Albert Einstein College, Bronx, NY; <sup>5</sup>IROA Technologies, Ann Arbor, MI
- TP 189 **Metabolomic Profiling of Biofluids Using Laser Desorption Ionization on Nanopost Array Devices (NAPAchips)**; Trust Razunguzwa; Heather Anderson; Nicholas Morris; Matthew Powell; Protea Biosciences, Inc., Morgantown, WV
- TP 190 **Untargeted Metabolic Profiling Distinguishes Gene-by-Diet "Metabotypes" at the Tissue Level in Mice**; Ann Wells<sup>1</sup>; William Barrington<sup>2</sup>; David Threadgill<sup>2</sup>; Arnold Saxton<sup>1</sup>; Stephen Dearth<sup>1</sup>; Shawn Campagna<sup>1</sup>; Brynne Voy<sup>1</sup>; <sup>1</sup>University of Tennessee-Knoxville, Knoxville, TN; <sup>2</sup>Texas A&M University, College Station, TX
- TP 191 **Metabolomic Analysis of Lung Epithelial Cells using Ion Mobility-Mass Spectrometry**; James C. Poland; M. Ray Keller; Stacy D. Sherrod; John A. Mclean; Vanderbilt University, Nashville, TN
- TP 192 **Metabolomic Profiling of Crustacean Neuroendocrine Tissues and Hemolymph by Capillary Electrophoresis-Electrospray Ionization-Mass Spectrometry**; Xuefei Zhong; Chuanzi Ouyang; Ling Hao; Lingjun Li; University of Wisconsin Madison, Madison, WI
- TP 193 **Profiling of Specialized Metabolites that Accumulate in Trichomes of *Solanum quitoense***; Steven Hurney; Michigan State University, East Lansing, MI
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- TP 195 **An Autonomous Workflow for Untargeted Metabolomics**; Baljit Ubhi<sup>1</sup>; Paul Benton<sup>2</sup>; Duane Rinehart<sup>2</sup>; Gary Siuzdak<sup>2</sup>; <sup>1</sup>SCIEX, Redwood City, CA; <sup>2</sup>Scripps Center for Metabolomics & Mass Spec, San Diego, CA
- TP 196 **Development of a Rapid LC-MS Method to Analyze Polar Metabolites in Complex Biological Samples; a Prelude to Kinetic Flux Profiling**; Jay Kirkwood; Corey Broeckling; Jordan Steel; Rushika Perera; Jessica Prenni; Colorado State University, Fort Collins, CO
- TP 197 **UPLC MS/MS-Driven Exploration of the Modulation of the Brain Metabolome by *Centella asiatica***; Parnian Lak<sup>1,2</sup>; Fereshteh Zandkarimi<sup>1</sup>; Nora Gray<sup>3</sup>; Christopher Harris<sup>3</sup>; Luisa Zini<sup>4</sup>; Brian Searle<sup>4</sup>; Jeff Morré<sup>1</sup>; Joseph Quinn<sup>3,5</sup>; Amala Soumyanath<sup>3</sup>; Jan F. Stevens<sup>2,6</sup>; Claudia Maier<sup>1,2</sup>; <sup>1</sup>Department of Chemistry, Oregon State University, Corvallis, OR; <sup>2</sup>Linus Pauling Institute, Oregon State University, Corvallis, OR; <sup>3</sup>Oregon Health and Science University, Portland, OR; <sup>4</sup>Proteome Software, Portland, OR; <sup>5</sup>Portland Veterans Affairs Medical Center, Portland, OR; <sup>6</sup>Pharmaceutical Sci. Oregon State University, Corvallis, OR
- TP 198 **Serum Metabolomic Profile of Diabetic Brazilian Population**; Kallyandra Padilha<sup>1</sup>; Gabriela Venturini<sup>1</sup>; Thiago Pires<sup>1</sup>; Celso Blatt<sup>2</sup>; Alexandre Pereira<sup>1</sup>; <sup>1</sup>Heart Institute, Sao Paulo, Brazil; <sup>2</sup>Agilent Technologies Brazil Ltda, Life Sciences &, São Paulo, SP
- TP 199 **Non-Lethal *in vivo* SPME Sampling of Fish Tissue in Combination with LC-HRMS Metabolites Profiling for Monitoring Internal Exposome**; Vincent Bessonneau<sup>1</sup>; Jennifer Ings<sup>2</sup>; Mark McMaster<sup>2</sup>; Richard Smith<sup>3</sup>; Leslie Bragg<sup>4</sup>; Mark Servos<sup>4</sup>; Janusz Pawliszyn<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Waterloo, Waterloo, Canada; <sup>2</sup>Environment Canada, Burlington, Canada; <sup>3</sup>Mass Spectrometry facility, University of Waterloo, Waterloo, Canada; <sup>4</sup>Department of Biology, University of Waterloo, Waterloo, Canada
- TP 200 **Application of Untargeted Metabolomics to Neurodegenerative Diseases**; He Huang; Alexandra Taraboletti; Leah Shriver; The University of Akron, Akron, Ohio
- TP 201 **CE-MS Analysis of Metabolites in Rare Cells Identified via MALDI-MS Profiling of Cell Populations**; Monika Makurath<sup>1</sup>; Ta-Hsuan Ong<sup>1</sup>; Troy Comi<sup>1</sup>; Stanislav Rubakhin<sup>2</sup>; Jonathan Sweedler<sup>1</sup>; <sup>1</sup>University of Illinois at Urbana-Champaign, Urbana, IL; <sup>2</sup>Beckman Institute, UIUC, Urbana, IL
- TP 202 **A Mass-Spectrometry-Based Metabolic Phenotyping Strategy to Investigate the Molecular Response to Ionizing Radiation**; Evagelia Laiakis<sup>2</sup>; Katrin Strassburg<sup>3</sup>; Steven Lai<sup>1</sup>; Robert Vreeken<sup>3,4</sup>; Thomas Hankemeier<sup>3</sup>; Jim

- Langridge<sup>1</sup>; Robert Plumb<sup>1</sup>; Albert Fornace Jr<sup>2</sup>; Giuseppe Astarita<sup>1,2</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Georgetown University, Washington, DC; <sup>3</sup>Leiden University, Leiden University, Netherlands; <sup>4</sup>Janssen Pharmaceutica, Discovery Sciences, Beerse, Belgium
- TP 203 **NanoLC-MS Reveals Chemical Differences Caused by Irradiation of Rodent Diets and may explain their Impact on Breast Cancer Risk**; Stephen Barnes; Landon Wilson; Ali Arabshahi; Xiangjin Cui; Samuel C Cartner; Casey M Morrow; Trenton Schoeb; Clinton J Grubbs; *University of Alabama at Birmingham, Birmingham, AL*
- TP 204 **Lipidomics Discovery for Serum Biomarkers**; Clementina Mesaros; Nathaniel W Snyder; Andrew J Worth; Ian A Blair; *University of Pennsylvania, Philadelphia, PA*
- TP 205 **isoMETLIN: A Database for Isotope-Based Metabolomics**; Kevin Cho<sup>1</sup>; Nathaniel Mahieu<sup>1</sup>; Winnie Uritboonthai<sup>2</sup>; Gary Siuzdak<sup>2</sup>; Gary J. Patti<sup>1</sup>; <sup>1</sup>Washington University School of Medicine, St. Louis, MO; <sup>2</sup>The Scripps Research Institute, La Jolla, CA
- TP 206 **Non-Targeted Metabolite Profiling of Dried Blood Spots in a Field Based Epidemiological Study**; Corey Broeckling; Jay Kirkwood; Maggie Clark; Jennifer Peel; Jessica Prenni; *Colorado State University, Fort Collins, CO*
- TP 207 **Enhanced Metabolite Profiling using Atmospheric Pressure Gas Chromatography (APGC) Coupled with Ion Mobility MS**; Manoj Ghaste<sup>2</sup>; Giuseppe Astarita<sup>3</sup>; Fulvio Mattivi<sup>2</sup>; Vladimir Shulaev<sup>1</sup>; <sup>1</sup>University of North Texas, Denton, TX; <sup>2</sup>Fondazione Edmund Mach, San Michele all'Adige, TN, Italy; <sup>3</sup>Waters Corporation, Milford, MA
- TP 208 **Metabolomic Characterization of Hepatocellular Carcinoma by Analysis of Human Liver Tissues Using LC/GC-MS**; Alessia Ferrarini; Cristina Di Poto; Rency Varghese; Mohammad R. Nezami Ranjbar; Habtom Resson; *Georgetown University, Lombardi Cancer Center, Washington, DC*
- TP 209 **Characterization of the Human Sweat Sub-Metabolome Using Dansyl Chloride Labeling and High-Resolution LC-MS**; Kevin Hooton; Liang Li; *University of Alberta, Edmonton, Canada*
- TP 210 **Effect of Mealybug Infestation on Grape Metabolomics**; Shabeer TP Ahammed<sup>1</sup>; Amala Udayakumar<sup>1</sup>; Akanksha Singh<sup>2</sup>; Manoj Pillai<sup>2</sup>; <sup>1</sup>National Research Centre for Grapes, Pune, Maharashtra, India; <sup>2</sup>SCIEX, 121, Udyog Vihar Phase IV, Gurgaon, Haryana, INDIA
- TP 211 **Optimized LC-MS Platform for Large-Scale Untargeted Metabolic Profiling of Human Urine and Plasma**; Kevin Contrepois; Lihua Jiang; Michael Snyder; *Stanford University, Stanford, California*
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- TP 213 **Development of Chemical Isotope Labeling LC-MS for Comparative Metabolomic Analysis of Yeast Cultured with and without Nitrogen Limitation**; Xian Luo; Liang Li; *Edmonton, Canada*
- TP 214 **Single-cell Mass Spectrometry Reveals Cell Heterogeneity in the 16-cell Frog (*Xenopus laevis*) Embryo**; Rosemary Onjiko; Sally A. Moody; Peter Nemes; *George Washington University, Washington, DC*
- TP 215 **Detection of Novel Biomarkers of Drug Toxicity Using Exploratory and Targeted Micro Scale LC/MS Analysis: A Metabolic Phenotyping Approach**; Robert Plumb<sup>1,2</sup>; Ian Wilson<sup>1,2</sup>; <sup>1</sup>Imperial College, London, UK; <sup>2</sup>Imperial College, London, UK
- TP 216 **Metabolomic Profiling in Breast Cancer Applying Micro-Sampling of Biological Fluids and Analysis by Gas Chromatography-Mass Spectrometry**; Monica P. Cala Molina; Roland J.W. Meesters; *Universidad de los Andes, Bogota D.C., COLOMBIA*
- TP 217 **Investigation of Gut Microbiota on Xanthohumol Metabolism Using High Resolution Mass Spectrometry with Ion Mobility and MS<sup>E</sup> Data Collection Techniques**; Liping Yang<sup>1</sup>; Fereshteh Zandkarimi<sup>1</sup>; Elahe Esfandiari<sup>2,3</sup>; Jeffrey Morr  <sup>1</sup>; Adrian Gombart<sup>2,3</sup>; Natalia Shulzhenko<sup>4</sup>; Jan Stevens<sup>2,5</sup>; Claudia Maier<sup>1,2</sup>; <sup>1</sup>Department of Chemistry, Oregon State University, Corvallis, OR; <sup>2</sup>Linus Pauling Institute, Oregon State University, Corvallis, OR; <sup>3</sup>Biochemistry & Biophysics, Oregon State University, Corvallis, OR; <sup>4</sup>Veterinary Medicine, Oregon State University, Corvallis, OR; <sup>5</sup>Pharmaceutical Sciences, Oregon State University, Corvallis, OR
- TP 218 **Shotgun Metabolome Profiling of a Yeast Knock-Out Library Using a GC-Orbitrap Mass Spectrometer**; Matthew Rush<sup>1</sup>; Nicholas Kwiecien<sup>1</sup>; Jonathan Stefely<sup>1</sup>; Alex Hebert<sup>1</sup>; Adam Jochem<sup>2</sup>; Michael S. Westphall<sup>1</sup>; David Pagliarini<sup>1</sup>; Scott Quarmby<sup>2</sup>; Jason Cole<sup>2</sup>; John Voss<sup>2</sup>; Joshua J. Coon<sup>1</sup>; <sup>1</sup>University of Wisconsin, Madison, WI; <sup>2</sup>Thermo Fisher Scientific, Austin, TX
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- TP 220 **Treasure Hunt for Novel Bioactive Compounds at Submarine Geothermal Chimneys in N-Iceland Utilizing UPLC-QTOF**; Eydis Einarsdottir<sup>1,2</sup>; Finnur F. Eiriksson<sup>1,2</sup>; HongBing Liu<sup>1</sup>; Sesselja Omarsdottir<sup>1</sup>; Margr  t Thorsteinsdottir<sup>1,2</sup>; <sup>1</sup>University of Iceland, Reykjavik, Iceland; <sup>2</sup>ArcticMass, Reykjavik, Iceland
- TP 221 **Comprehensive Analysis of in-vivo metabolites using MS/MSall SWATH<sup>TM</sup> Acquisition and Online Information Dependent Analysis Based on High Resolution Mass Spectrometry**; Liang Li<sup>1</sup>; Xiaoyan Chen<sup>1</sup>; Dafang Zhong<sup>1</sup>; Ting Liu<sup>2</sup>; Suma Ramagiri<sup>2</sup>; Cheng Yang<sup>2</sup>; Kerong Zhang<sup>2</sup>; Wei Cheng<sup>2</sup>; <sup>1</sup>Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai, China; <sup>2</sup>SCIEX Asia Pacific Application Support Center, Shanghai, China
- TP 222 **Development of an Algorithm for the Structure Elucidation of Unknown Small Molecules Drugs**; Tatiana Radchenko<sup>1</sup>; Fabien Fontaine<sup>2,3</sup>; Ismael Zamora<sup>2</sup>; <sup>1</sup>University Pompeu Fabra, BARCELONA, SPAIN; <sup>2</sup>Lead Molecular Design S.L., Sant Cugat de Valles, Spain; <sup>3</sup>Molecular Discovery, London, UK
- TP 223 **Profiling the Effects of Menadione and 2,3-Dimethoxy-1,4-Naphthoquinone on Redox Status by LC-MS**; Dylan Marchione; Andrew Worth; Clementina Mesaros; Nathaniel Snyder; Ian Blair; *University of Pennsylvania, Philadelphia, PA*
- TP 224 **MassMetasite and Webmetabase for Metabolite Profiling of Radiolabeled Samples: Automation of Data Analysis in Development Studies**; Ismael Zamora<sup>1</sup>; Fabien Fontaine<sup>2</sup>; Blanca Serra<sup>2</sup>; Caroline Woodward<sup>3</sup>; Natasha Penner<sup>3</sup>; <sup>1</sup>Lead Molecular Design, S.L., Sant Cugat Del Valles, SPAIN; <sup>2</sup>Molecular Discovery, Ltd, London, UK; <sup>3</sup>Biogen Idec, Cambridge, MA
- TP 225 **Comparison of Glatiramer Acetate Through Differential Mass Spectrometry**; Sarah Rogstad; Eric Pang; Cynthia Sommers; David Keire; Michael Boyne; *US FDA, Silver Spring, MD*



- TP 226 **Software-Aided Workflow for Investigation of Catabolic Degradation Products during Peptide Therapeutics Compound Optimization**; Eva Duchoslav; Jinal Patel; Suma Ramagiri; *SCIEX, Concord, Canada*
- TP 227 **Characterization of KCN-Trapped Reactive Metabolites of Anticancer Tyrosine Kinase Inhibitors in *in-vitro* RLM Preparations Using Tandem Mass Spectrometry**; Adnan A. Kadi<sup>1</sup>; Mohamed W. Attwa<sup>1</sup>; Hany W. Darwish<sup>1,2</sup>; Sawsan M. Amer<sup>2</sup>; <sup>1</sup>College of Pharmacy, King Saud University, Riyadh, Saudi Arabia; <sup>2</sup>College of Pharmacy, Cairo University, Cairo, Egypt
- TP 228 **LC-MS/MS Identification of *in vitro* Metabolites of the Alkaloid Govaniadine Produced by Rat and Human Liver Microsomes**; Lucas Maciel Mauriz Marques; Anderson Rodrigo Moraes de Oliveira; Ricardo Vessecchi; Norberto Peoporine Lopes; *University of Sao Paulo, Ribeirao Preto, Brazil*
- TP 229 **Investigation of *in vitro* metabolism of Sulfur- and Chlorine-Containing Drug Using Capillary UPLC Coupled to ICP-MS and ESI-LTQ/Orbitrap**; Heng-Keang Lim; Dewakar Sangaraju; Rhys Salter; *Janssen Pharmaceutical R&D, Spring House, PA*
- TP 230 **Tissue-Engineered Long Term Hepatocyte Co-Culture Model and Data Independent Mass Spectrometry Acquisition to Identify Multi Generation Metabolites**; Yvonne Schaus<sup>1</sup>; Suma Ramagiri<sup>2</sup>; Gary Impey<sup>2</sup>; Jack McGeehan<sup>1</sup>; Vince Zurawski<sup>1</sup>; <sup>1</sup>Hepregen, Boston, MA; <sup>2</sup>SCIEX, Concord, Canada
- TP 231 **Evaluation of High Resolution Mass Spectrometry for Integrated Quantitative and Qualitative Bioanalysis Following Oral Administration of Loratadine to Rats**; Quintin Ferraris; Jui Chaugule; Khushbu Gajjar; Dil Ramanathan; *Kean University, Union, NJ*
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- TP 233 **Comprehensive Metabolite Detection by Utilising both Positive and Negative Ionization on an Integrated Microfluidic-Ion Source with CCS Measurements**; Richard Gallagher<sup>1</sup>; Christine Pattison<sup>1</sup>; Kathryn Pickup<sup>1</sup>; John Chipperfield<sup>2</sup>; Mike McCullagh<sup>2</sup>; Jim Murphy<sup>3</sup>; David Douce<sup>2</sup>; <sup>1</sup>AstraZeneca, Macclesfield, UK; <sup>2</sup>Waters (MS Technologies), Wilmslow, UK; <sup>3</sup>Waters, Milford, MA
- TP 234 **Identification of Osthole Metabolites in Rat Liver Microsomes by Heart-Cut Two-Dimensional-Liquid Chromatography/ Q-TOF Mass Spectrometry System**; Guoqiang Liu<sup>1</sup>; Qian Liu<sup>2</sup>; Yue Song<sup>1</sup>; Shan-An Chan<sup>3</sup>; <sup>1</sup>Agilent Technology, Inc. Shanghai, Shanghai, China; <sup>2</sup>Shanghai Nature Standard R&D and Biotech Co., Ltd, Shanghai, China; <sup>3</sup>Agilent Technology, Inc. Taipei, Taiwan
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- TP 236 **Polar Lipid Compositions of Different Algal Species Obtained by LC Negative ESI 14.5 T FT-ICR Mass Spectrometry**; Peilu Liu<sup>1</sup>; Yuri Corilo<sup>1</sup>; Greg T. Blakney<sup>1</sup>; Alan G. Marshall<sup>1,2</sup>; <sup>1</sup>ICR Program at NHMFL, Tallahassee, FL; <sup>2</sup>Department of Chemistry and Biochemistry, FSU, Tallahassee, FL
- TP 237 **Development of a High-Throughput, Untargeted UPLC-MS Lipidomics Platform for Mammalian Biofluids: Application for Identifying Predictive Disease Markers in Dairy Cows**; Fereshteh Zandkarimi<sup>1</sup>; Gerd Bobe<sup>2,3</sup>; Claudia S. Maier<sup>1,2</sup>; <sup>1</sup>Department of Chemistry, Oregon State University, Corvallis, OR; <sup>2</sup>Linus Pauling Institute, Oregon State University, Corvallis, OR; <sup>3</sup>Animal and Rangeland Sci., Oregon State University, Corvallis, OR
- TP 238 **MALDI-IMS Detects Differential White Matter Degeneration-Associated Lipid Profiles in Rat Models of Chronic Alcohol, Tobacco Nitrosamine, or Both Exposures**; Emine Yalcin<sup>1,2</sup>; Kavin Nunez<sup>1,2</sup>; Ming Tong<sup>1,2</sup>; Shannon Cornett<sup>3</sup>; Suzanne de la Monte<sup>1,2</sup>; <sup>1</sup>Liver Research Center, Rhode Island Hospital, Providence, RI; <sup>2</sup>Alpert Medical School of Brown University, Providence, RI; <sup>3</sup>Bruker Daltonics, Billerica, MA
- TP 239 **Matrix-Assisted Ionization-Mass Spectrometry Enables Cardiolipin Characterization Directly From Intact Mitochondrial Membranes**; Christian Reynolds; Jessica DeLeeuw; Corinne Lutomski; Thomas Sanderson; Karin Przyklenk; Sarah Trimpin; *Wayne State University, Detroit, MI*
- TP 240 **Rapid In-Depth Regioisomer Focused Lysophospholipidomics of Human Serum by Online Supercritical Fluid Extraction-Supercritical Fluid Chromatography Tandem Mass Spectrometry**; Yoshihiro Izumi<sup>1,2</sup>; Yasuhiro Funada<sup>3</sup>; Uchikata Takato<sup>3</sup>; Yosuke Iwata<sup>3</sup>; Masami Tomita<sup>3</sup>; Nishimura Masayuki<sup>4</sup>; Kim H Ekroos<sup>5</sup>; Takeshi Bamba<sup>1,2</sup>; <sup>1</sup>Medical Institute of Bioregulation Kyushu Univ., Fukuoka, Japan; <sup>2</sup>Grad. Sch. Eng., Osaka Univ., Suita, Japan; <sup>3</sup>Shimadzu Co., Kyoto, Japan; <sup>4</sup>Shimadzu Marketing Center, Columbia, U.S.A.; <sup>5</sup>Zora Biosciences Oy, Espoo, Finland
- TP 241 **Targeted and Untargeted Lipidomics using an Integrated Microfluidics Mass Spectrometry Technology**; Steven Lai; Paul Rainville; Angela Doneanu; Jay Johnson; James Murphy; Robert Plumb; Giuseppe Astarita; *Waters Corporation, Milford, MA*
- TP 242 **A Novel Lipid Screening Platform Allowing a Complete Solution for Lipidomics Research**; Alex Conner<sup>1</sup>; Baljit K Ubhi<sup>3</sup>; Eva Duchoslav<sup>4</sup>; Leo Wang<sup>3</sup>; Paul RS Baker<sup>2</sup>; Steven Watkins<sup>1</sup>; <sup>1</sup>Lipomics, Sacramento, CA; <sup>2</sup>SCIEX, Framingham, MA; <sup>3</sup>SCIEX, Redwood City, CA; <sup>4</sup>SCIEX, Toronto, ON
- TP 243 **Global Characterization and Quantitation of Lipid C=C Isomers in Tissues by On-Line Photochemical Derivatization and Mass Spectrometry**; Xiaoxiao Ma; Leelyn Chong; Zheng Ouyang; Yu Xia; *Purdue University, West Lafayette, IN*
- TP 244 **Laser Ablation and Droplet Capture in the Visible Range: A New Tool for Spatially Resolved Lipidomics and Proteomics**; Benoit Fatou<sup>1,2</sup>; Maxence Wiszorski<sup>1</sup>; Cristian Focsa<sup>2</sup>; Michel Salzet<sup>1</sup>; Michael Ziskind<sup>2</sup>; Isabelle Fournier<sup>1</sup>; <sup>1</sup>PRISM Laboratory INSERM U 1192, University of Lille 1, Villeneuve d'Ascq, France; <sup>2</sup>PhLAM Laboratory, UMR 8523, University of Lille 1, Villeneuve d'Ascq, France
- TP 245 **Retinoic Acid Analysis with Differential Mobility Mass Spectrometry for Improved Selectivity and Sensitivity**; Leo (Jinyuan) Wang<sup>1</sup>; Jace W. Jones<sup>2</sup>; Maureen A. Kane<sup>2</sup>; Pauk R.S. Baker<sup>1</sup>; <sup>1</sup>AB SCIEX, Redwood City, CA; <sup>2</sup>University of Maryland, School of Pharmacy, Baltimore, MD
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- TP 247 **Method Development for the Analysis of Endogenous Steroids by UPC<sup>2</sup>-MS/MS**; Neil de Kock; Kumari Ubhayasekera; Jonas Bergquist; *Department of Chemistry–BMC, Uppsala University, Uppsala, Sweden*
- TP 248 **Bacteria Identification by Laser Desorption Ionization Mass Spectrometry (LDI-MS) – Enhancement of Signal Consistence using Amorphous Silicon (a-Si) Thin Films**; Sohee Yoon<sup>1</sup>; Shin Hye Kim<sup>1</sup>; Jeong Hee Moon<sup>2</sup>; Kyung Joong Kim<sup>1</sup>; Tae Geol Lee<sup>1</sup>; <sup>1</sup>KRISS, Daejeon, Republic of Korea; <sup>2</sup>KRIBB, Daejeon, Republic of Korea

- TP 249 **The Effects of *Foxn1* Silencing on the Skin Mice Lipidome**; Justine Lanzini<sup>1</sup>; Delphine Dargère<sup>1</sup>; Anne Regazzetti<sup>1</sup>; Abdellah Tebani<sup>1</sup>; Olivier Laprèvote<sup>1,2</sup>; Nicolas Auzeil<sup>1</sup>; <sup>1</sup>UMR CNRS 8638, Université Paris Descartes, Paris, France; <sup>2</sup>AP-HP, Hôpital Lariboisière, Paris, France
- TP 250 **Supercritical Fluid Chromatography - Mass Spectrometry and Lipids – A Perfect Marriage**; John Langley<sup>1</sup>; Julie Herniman<sup>1</sup>; Caroline Sayer<sup>1</sup>; Joost Brandsma<sup>2</sup>; Tom Sutton<sup>2</sup>; Waraporn Ratsameepakai<sup>1</sup>; Tim Jenkins<sup>3</sup>; <sup>1</sup>Chemistry, University of Southampton, Southampton, UK; <sup>2</sup>Medicine, University of Southampton, Southampton, UK; <sup>3</sup>Waters Corporation, Wilmslow, UK
- TP 251 **Chromatographic Separation of Phosphatidylcholine Isomers on a UHPLC-MS Timeframe with Quadrupole Orbitrap Mass Spectrometer Detection**; Josef Ruzicka<sup>1</sup>; David A. Peake<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, Somerset, NJ; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- TP 252 **Comprehensive Lipid Analysis by MALDI Imaging and Spatially Resolved MS/MS Sequencing in Three Dimensional Cell Culture Models of Colorectal Carcinoma**; Eric Weaver<sup>1</sup>; Andrew Palmer<sup>2,3</sup>; Michael Becker<sup>4</sup>; Jens Fuchser<sup>4</sup>; Theodore Alexandrov<sup>2,5</sup>; Amanda B. Hummon<sup>1</sup>; <sup>1</sup>University of Notre Dame, Notre Dame, IN; <sup>2</sup>EMBL Heidelberg, Heidelberg, Germany; <sup>3</sup>University of Bremen, Bremen, Germany; <sup>4</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>5</sup>SCILS, Bremen, Germany
- TP 253 **An Interactive Software for LC-MS/MS Lipid Identification and Quantitation**; Kevin L. Crowell<sup>1</sup>; Yong J. Kil<sup>1</sup>; Marshall W. Bern<sup>1</sup>; Chris H. Becker<sup>1</sup>; Jennifer E. Kyle<sup>2</sup>; Richard D. Smith<sup>2</sup>; Thomas O. Metz<sup>2</sup>; <sup>1</sup>Protein Metrics Inc., San Carlos, California; <sup>2</sup>Pacific Northwest National Laboratory, Richland, WA
- TP 254 **A Comprehensive Data-Independent Lipidomic Survey in Serum after Chronic Exposure to Strontium-90 *in vivo***; Maryam Goudarzi<sup>1</sup>; Waylon Weber<sup>2</sup>; Tytus Mak<sup>3</sup>; Juijung Chung<sup>1</sup>; Melanie Doyle-Eisele<sup>2</sup>; Dunstana Melo<sup>2</sup>; Steve Strawn<sup>1</sup>; David Brenner<sup>4</sup>; Raymond Guilmette<sup>2</sup>; Albert Fornace Jr. <sup>1</sup>; <sup>1</sup>Georgetown University, Washington Dc, DC; <sup>2</sup>Lovelace Respiratory Research Institute, Albuquerque, NM; <sup>3</sup>National Institute of Standards and Technology, Gaithersburg, MD; <sup>4</sup>Columbia University, New York, NY
- TP 255 **Application of an Integrated Ion Cyclotron Based High Resolution Lipidomics Platform on RORy Ligand Search**; Harald Koefeler<sup>1</sup>; Bettina Meissburger<sup>2,5</sup>; Troetzmueller Martin<sup>1</sup>; Alexander Triebel<sup>1</sup>; Alexander Fauland<sup>3</sup>; Juergen Hartler<sup>1</sup>; Christian Wolfrum<sup>2</sup>; <sup>1</sup>Medical University Graz, ZMF, Graz, AUSTRIA; <sup>2</sup>Eidgenössische Technische Hochschule, Zürich, Switzerland; <sup>3</sup>Karolinska Institutet, Stockholm, Sweden; <sup>4</sup>Graz University of Technology, Graz, Austria; <sup>5</sup>DKFZ, Heidelberg, Germany
- TP 256 **Profiling and Quantitation of Globosides (Gb4) in Biological Samples Using Ultra-Fast Mass Spectrometry**; Ruth Gordillo<sup>1</sup>; William L. Holland<sup>1</sup>; Benjamin J. Figard<sup>2</sup>; Erin McAllister<sup>2</sup>; David Jorissen<sup>2</sup>; Philipp E. Scherer<sup>1</sup>; <sup>1</sup>UTSW Medical Center, Touchstone Diabetes Center, Dallas, Texas; <sup>2</sup>Shimadzu Scientific Instruments, Columbia, MD
- TP 257 **HR/AM Mass Spectrometry Methodologies for Rapid Screening and Comprehensive Studies of Lipid Deposition Correlation to Contact Lens Properties**; Andrew J. Hotelling<sup>1</sup>; William Nichols<sup>2</sup>; <sup>1</sup>Bausch + Lomb, Rochester, NY; <sup>2</sup>Mass2Charge Consulting LLC, Romulus, NY
- TP 258 **Lipidomic Profiling of Gut commensal *Bacteroidales* and Elucidating Immunomodulatory Sphingolipid Biosynthesis**; Sungwhan Oh; Naama Geva-Zatorsky; Wen Zheng; Dennis Kasper; Harvard Medical School, Boston, MA
- TP 259 **Comprehensive Two-Dimensional HPLC Analysis Coupled with Mass Spectrometric Detection and Informative Data Processing for Lipids Analysis**; Tetsuo Iida<sup>1</sup>; Yoshiyuki Watabe<sup>1</sup>; Daisuke Nakayama<sup>1</sup>; Kanya Tsujii<sup>1</sup>; Saki Ueda<sup>1</sup>; Kenichiro Tanaka<sup>2</sup>; Tadayuki Yamaguchi<sup>1</sup>; Junichi Masuda<sup>1</sup>; Yoshihiro Hayakawa<sup>1</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>Shimadzu Scientific Instruments, Inc., Columbia
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- TP 262 **Lipidomics Approach Reveals Potential Xanthohumol Anti-Obesity Mechanism through Triglycerides Identification and Fatty Acids Composition**; Jaewoo Choi<sup>1</sup>; Cristobal L. Miranda<sup>1,2</sup>; Hyi-Seung Lee<sup>1,3</sup>; Hye-Kyeong Kim<sup>1,4</sup>; Jan F. Stevens<sup>1,2</sup>; <sup>1</sup>Linus Pauling Institute, Oregon State University, Corvallis, Oregon; <sup>2</sup>College of Pharmacy, Oregon State University, Corvallis, Oregon; <sup>3</sup>Korea Institute of Ocean Science and Technology, Ansan, South Korea; <sup>4</sup>The Catholic University of Korea, Bucheon, South Korea
- TP 263 **Lipid Profiling Analysis of Liver Tissues between Obesity-Prone and Obesity-Resistant Mice under High Fat Diet**; Sunhee Jung<sup>1,2</sup>; Miso Nam<sup>1,2</sup>; Youngae Jung<sup>1</sup>; Do Hyun Ryu<sup>2</sup>; Geum-Sook Hwang<sup>1,3</sup>; <sup>1</sup>Korea Basic Science Institute, Seoul, Republic of Korea; <sup>2</sup>Sungkyunkwan University, Suwon, Republic of Korea; <sup>3</sup>Graduate School of Analytical Science and Technol, Daejeon, Republic of Korea
- TP 264 **Fetal Sex-dependent Effects of Maternal Obesity on Dysregulation of Lipid Metabolic Pathways in the Placenta**; Xiaoli Gao; Sribalashubashini Muralimanoharan; Susan T Weintraub; Leslie Myatt; Alina Maloyan; UT Health Science Center at San Antonio, San Antonio, TX
- TP 265 **Lipidomics of Marine Microorganisms under Stress. Solving the Needle / Haystack Problem with a Large Database and Open-Source Software**; Helen Fredricks; James Collins; Bethanie Edwards; Benjamin Van Mooy; Woods Hole Oceanographic Institution, Woods Hole, MA
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- TP 267 **High Resolution LC-MS Demonstrates Serum Triglyceride Composition is Affected Qualitatively and Quantitatively by Interactions of Dietary Fat and Carbohydrate**; Bruce Kristal<sup>1,2</sup>; Irina Stavrovskaya<sup>1</sup>; Susan Bird<sup>1,3</sup>; Vasant Marur<sup>1</sup>; Caryn Porter<sup>1,4</sup>; <sup>1</sup>Brigham + Women's Hospital, Boston, MA; <sup>2</sup>Harvard Medical School, Boston, MA; <sup>3</sup>ThermoFisher (Current), Boston, MA; <sup>4</sup>Mass General Hospital (Current), Boston, MA
- TP 268 **Can "Classic" Lipid Profiling Data on a QQQ Justify Diving into a Full Profile of the Sphingolipid Pool?** Todd Williams; Lei Jiang; Elias Michaelis; Marylou Michaelis; University of Kansas, Lawrence, KS
- TP 269 **Lipidomic Profiling of Plasma from Patients with Atrial Fibrillation by UPLC/Q-TOF MS**; Youngae Jung<sup>1</sup>; Doo-Hae Lee<sup>1,2</sup>; Geum-Sook Hwang<sup>1,2</sup>; <sup>1</sup>KBSI Western Seoul Center, Seoul, Republic of Korea; <sup>2</sup>GRAST in Chungnam University, Daejeon, Republic of Korea





- TP 270 **Development of a Comprehensive Monitoring Method of Lipid Mediator Species for Human Plasma Profiling;** Masaki Yamada<sup>1,2</sup>; Yoshihiro Kita<sup>1</sup>; Takahiro Kohira<sup>1,3</sup>; Suzumi M. Tokuoka<sup>1</sup>; Takao Shimizu<sup>1,4</sup>; <sup>1</sup>The University of Tokyo, Tokyo, Japan; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan; <sup>3</sup>Japanese Red Cross Society, Tokyo, Japan; <sup>4</sup>National Center for Global Health and Medicine, Tokyo, Japan
- TP 271 **Comprehensive and Quantitative Analysis of Fatty Acids in Biological Samples by Gas Chromatography-Mass Spectrometry;** Jaeman Byun; Anna Mathew; Subramaniam Pennathur; *University of Michigan, Ann Arbor, MI*
- TP 272 **Lipidomic Profiling of Plasma from Radiation Animal Models;** Jace W. Jones<sup>1</sup>; Claire L. Carter<sup>1</sup>; Gregory Tudor<sup>2</sup>; Alexander Bennett<sup>1</sup>; Ann Farese<sup>1</sup>; Catherine Booth<sup>2</sup>; Thomas J. MacVittie<sup>1</sup>; Maureen A. Kane<sup>1</sup>; <sup>1</sup>University of Maryland, Baltimore, MD; <sup>2</sup>Epistem Ltd., Manchester, UK
- TP 273 **LC-MS/MS Profiling of Gangliosides in Mouse Retina;** Ashta Lakshmi Prasad Gobburu<sup>1</sup>; Dr. Denise M. Inman<sup>2</sup>; Dr. Renliang Zhang<sup>3</sup>; Dr. Belinda Willard<sup>3</sup>; Dr. David J Anderson<sup>1</sup>; <sup>1</sup>Cleveland State University, Department of Chemistr, Cleveland, OHIO; <sup>2</sup>Northeast Ohio Medical University, Rootstown, Ohio; <sup>3</sup>Cleveland Clinic, Cleveland, Ohio
- TP 274 **Comparison of LC-Orbitrap-MS with Infusion-based Shotgun MS for Lipidomic Profiling;** Russell Pickford<sup>1</sup>; Magda Montgomery<sup>1</sup>; Simon Brown<sup>2</sup>; Todd W Mitchell<sup>2</sup>; Nigel Turner<sup>1</sup>; <sup>1</sup>University of New South Wales, Sydney, Australia; <sup>2</sup>University of Wollongong, Wollongong, Australia
- TP 275 **Lipid Data Analyzer 2: Flexible and Automatic Identification of Lipid Structures in High-Throughput LC-MS<sup>n</sup> Data from Various Instruments;** Juergen Hartler<sup>1,2</sup>; Alexander Triebel<sup>3</sup>; Martin Troetzmueller<sup>3</sup>; Andreas Ziegler<sup>1</sup>; Gerald N. Rechberger<sup>4</sup>; Friedrich Spener<sup>4</sup>; Harald C. Koefeler<sup>3</sup>; Gerhard G. Thallinger<sup>1,2</sup>; <sup>1</sup>Bioinformatics, IKD, Graz University of Technology, Graz, Austria; <sup>2</sup>Omics Center Graz, Graz, Austria; <sup>3</sup>ZMF, Medical University of Graz, Graz, Austria; <sup>4</sup>Institute of Molecular Biosciences, University of, Graz, Austria
- TP 276 **Determining the Potential Underlying Mechanism of Anesthetic-Induced Neurotoxicity in the Developing Monkey Brain Using Shotgun Lipidomics;** Jessica Frisch-Daiello<sup>1</sup>; Fang Liu<sup>2</sup>; Cheng Wang<sup>2</sup>; Xianlin Han<sup>1</sup>; <sup>1</sup>Sanford-Burnham Medical Research Institute, Orlando, FL; <sup>2</sup>National Center for Toxicological Research - FDA, Jefferson, AR
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- TP 278 **SIFT-MS - a 24/7 Analytical Technique;** Daniel Milligan<sup>1</sup>; John Gray<sup>1</sup>; Vaughan Langford<sup>1</sup>; Murray McEwan<sup>2</sup>; <sup>1</sup>Syft Technologies Ltd, Christchurch, New Zealand; <sup>2</sup>University of Canterbury, Christchurch, New Zealand
- TP 279 **Automation of Calibration Curve Redaction for Absolute Quantitation by LC/MS;** Lyle Burton; Michael J. Y. Jarvis; *SCIEX, Concord, Ontario*
- TP 280 **Highly Sensitive Quantitative Analysis of Amoxicillin and Clavulanic Acid from Plasma Using LC/MS/MS;** Deepti Bhandarkar; Rashi Kochhar; Shailendra Rane; Shruti Raju; Shailesh Damale; Ajit Datar; Pratap Rasam; Jitendra Kelkar; *Shimadzu Analytical (India) Pvt. Ltd., Mumbai, INDIA*
- TP 281 **Quantification of Total and Free Metal-Based Oncology Drugs Using ICP-MS Methods for Clinical and Pre-Clinical Studies;** Nicole Greer; Xuefei Guo; Elise Snider; Yong-Xi Li; *Medpace Bioanalytical Laboratories, Cincinnati, OH*
- TP 282 **The Control of the Formation and Degradation of Omega-3 Ethyl Esters in Human Plasma;** Luc Bouchard; Genevieve Emond; François Viel; Philippe Bélanger; Nadine Boudreau; Ann Lévesque; *inVentiv Health Clinical, Québec, Canada*
- TP 283 **Low level quantitation of Fluticasone and Salmeterol from plasma using LC/MS/MS;** Shruti Raju; Rashi Kochhar; Shailendra Rane; Deepti Bhandarkar; Shailesh Damale; Ajit Datar; Jitendra Kelkar; Pratap Rasam; *Shimadzu Analytical (India) Pvt. Ltd., Mumbai, INDIA*
- TP 284 **Efficient Method for the Analysis of Ticagrelor and its Metabolite AR-C124910XX in Human EDTA K2 Plasma by LCMSMS;** Pierre-Yves Caron; François Viel; Nadine Boudreau; Ann Lévesque; *inVentiv Health Clinical, Québec, Canada*
- TP 285 **Hydrolysis Conditions Investigation for Analysis of Total Dabigatran in Human Plasma;** Pierre-Yves Caron; Nancy Lampron; François Viel; Nadine Boudreau; Ann Lévesque; *inVentiv Health Clinical, Québec, Canada*
- TP 286 **Using Surrogate Matrices for the Determination of Sodium and Potassium in Human Urine using ICP-MS;** Patrice Lantin; François Viel; Nadine Boudreau; Ann Lévesque; *inVentiv Health Clinical, Québec, Canada*
- TP 287 **Determination of Selenomethionine in Animal Feed by High Performance Liquid Chromatography – Inductively Coupled Plasma – Mass Spectrometry;** Paula Fisher; *Novus International, St. Charles, MO*
- TP 288 **Stabilizing Frozen Human Serum Liposomal Amphotericin B Sample to Prevent Disruption of liposomes;** Jason Bilodeau; François Viel; Nadine Boudreau; Ann Lévesque; *inVentiv Health Clinical, Québec, Canada*
- TP 289 **An Ultra-Sensitive Method for Femtogram Level Detection of Dexamethasone in Human Plasma using LC/MS/MS;** Jason Bilodeau; François Viel; Nadine Boudreau; Ann Lévesque; *inVentiv Health Clinical, Québec, Canada*
- TP 290 **Development and Validation of an LC-MS/MS Method for the Quantification of Hydroxypropyl  $\beta$ -Cyclodextrin in Human Plasma;** Chun-Yi Wu<sup>1</sup>; Ihid C. Leao<sup>2</sup>; James E. K. Hildreth<sup>2</sup>; Ai-Ming Yu<sup>1</sup>; <sup>1</sup>UC Davis PK/PD Bioanalytical Core Facility, Sacramento, CA; <sup>2</sup>Dept of Molecular and Cellular Biology, UC Davis, Davis, CA
- TP 291 **Complex Quantification of modified  $\beta$ -Cyclodextrin in Human EDTA K2 Plasma using Monolithic Column by LCMSMS;** Guy Havarid; François Viel; Nadine Boudreau; Ann Lévesque; *inVentiv Health Clinical, Québec, Canada*
- TP 292 **Headspace Gas Chromatography-Mass Spectrometry Analysis of Volatile Compounds in Biological Samples;** Wanqing Lu; Aiping Zhu; Nelson Santiago; Yong-xi Li; *Medpace Bioanalytical Laboratories, Cincinnati, OH*
- TP 293 **A Simple LC-MS/MS Method for Determination of Fluticasone Propionate and Salmeterol Xinafoate in Human Plasma at pg/mL Level;** Huafang Jiang; Peipei Zhang; Hongxia Chai; Xiaohang Shen; Xin Zhang; Wenzhong Liang; *WuXi AppTec (Shanghai) Co. Ltd., Shanghai, China*
- TP 294 **Determination of Digoxin in Human Urine Using High Performance Liquid Chromatography-mass Spectrometry;** Wuyi Zha; Runlan Huo; Mohamed Osman; Jinn Wu; Xinping Fang; *XenoBiotic Laboratories, Inc., WuXi AppTec, Inc, Plainsboro Township, NJ*

- TP 295 **A Sensitive LC-MS/MS Method for Quantitation of Buprenorphine and Norbuprenorphine in Human Plasma;** Xinping Fang; Dawei Zhou; Shu Zhang; Jinn Wu; *XenoBiotic Laboratories, Inc., WuXi AppTec, Inc., Plainsboro, NJ*
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- TP 297 **Impurity Characterisation of the Fungicide Flutriafol using Liquid Chromatography and Time of Flight MS Detection to Aid Pesticide Product Registration;** Marian Twohig<sup>1</sup>; Oliver Burt<sup>2</sup>; Gordon Fujimoto<sup>3</sup>; Peter Lee<sup>1</sup>; John McCauley<sup>4</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Waters Corporation, Wilmslow, UK; <sup>3</sup>Waters Corporation, Beverly, MA; <sup>4</sup>Waters Corporation, New Castle, DE
- TP 298 **LC/MS/MS Analysis of Urinary Biomarkers of the Fungicide Pyrimethanil following Experimental Exposure in Humans;** Moosa Faniband; Eva Ekman; Margareta Littorin; Margareta Maxe; Bo A. Jönsson; Christian Lindh; *Lund University, Lund, Sweden*
- TP 299 **Highly Sensitive Determination of Acidic Pesticides Residues in Agricultural Commodities by Paired Ion Electrospray Ionization (PIESI) Mass Spectrometry;** Hongyue Guo<sup>1,2</sup>; Leah Riter<sup>1</sup>; Chad Wujcik<sup>1</sup>; Daniel Armstrong<sup>2</sup>; <sup>1</sup>Monsanto, St Louis, MO; <sup>2</sup>University of Texas at Arlington, Arlington, TX
- TP 300 **Novel Approach to Sample Preparation for Contaminant Analysis in Food using the Thomson eXtreme Filter Vials® by LC-MS/MS and GC-MS;** Samuel Ellis; Lisa Wanders; *Thomson Instrument Company, Oceanside, CA*
- TP 301 **Direct Determination of Trace Hormones in Drinking Water by Large Volume Injection at Sub ng/L Levels Using LC-MS/MS;** David R. Baker; Neil J Loftus; *Shimadzu, Manchester, UK*
- TP 302 **Supercritical Fluid Chromatography Triple-Quadrupole Mass Spectrometry: An Alternative to LC/MS/MS for High-Sensitivity and -Throughput Analysis of Multiresidue Pesticides;** Yoshihiro Izumi<sup>1,2</sup>; Eiichiro Fukusaki<sup>2</sup>; Takeshi Bamba<sup>1,2</sup>; <sup>1</sup>Medical Institute of Bioregulation, Kyushu Univ., Fukuoka, Japan; <sup>2</sup>Dept. Biotech., Grad. Sch. Eng., Osaka Univ., Osaka, Japan
- TP 303 **Structural Elucidation and Estimation of the Acute Toxicity of the Major UV-Visible Photoproduct of Fludioxonil – Detection in Grape Samples;** Yannick Lassalle; Édith Nicol; Christophe Genty; Sophie Bourcier; Stéphane Bouchonnet; *LCM UMR-9168, École Polytechnique, Palaiseau, France*
- TP 304 **Rapid Screening of the Potential Chemical Contaminants in Underground Water Using UHPLC-QTOF Mass Spectrometry;** Jing Guo<sup>1</sup>; Bing Du<sup>1</sup>; Meiling Lu<sup>2</sup>; Jerry Zweigenbaum<sup>3</sup>; Thomas Glauner<sup>4</sup>; Yeru Huang<sup>1</sup>; <sup>1</sup>Natl Res Center for Environ Anal Measurement, Beijing, China; <sup>2</sup>Agilent Technologies (China) Limited, Beijing, China; <sup>3</sup>Agilent Technologies US, Wilmington, DE; <sup>4</sup>Agilent Technologies GmbH, Waldbronn, Germany
- TP 305 **Direct Analysis of Pharmaceuticals and Personal Care Products (PPCPs) in Environmental Waters using a Newly Developed Triple Quadrupole Mass Spectrometer;** Jian-Zhong Li<sup>2</sup>; Michael Thurman<sup>4</sup>; Imma Ferrer<sup>4</sup>; Craig Marvin<sup>3</sup>; Anabel Fandino<sup>1</sup>; Na Pi Parra<sup>1</sup>; <sup>1</sup>Agilent Technologies, Inc., Santa Clara, CA; <sup>2</sup>Agilent Technologies, Inc., Beijing, China; <sup>3</sup>Agilent Technologies, Wilmington, DE; <sup>4</sup>University of Colorado, Boulder, Colorado
- TP 306 **Applications of a Novel, High Performance LC-MS/MS Ion Source;** Heather Gamble<sup>1</sup>; Sha Joshua Ye<sup>1</sup>; Ellie Majdi<sup>1</sup>; Donald Gamble<sup>2</sup>; <sup>1</sup>IONICS Mass Spectrometry Group, Bolton, ON; <sup>2</sup>St. Mary's University, Halifax, Canada
- TP 307 **Cross Validation between LDTD-MS/MS and LC-MS/MS for 5 Neonicotinoids Insecticides in Water;** Gregory Blachon; Alex Birsan; Serge Auger; Jean Lacoursière; Pierre Picard; *Phytronix Technologies, Inc., Quebec, QC*
- TP 308 **Development of Electrochemical Methods Capable of Mimicking Oxidative Degradation Pathway of Model Pharmaceuticals;** Marc-André Lecours; Gessie Brisard; Pedro A. Segura; *University of Sherbrooke, Sherbrooke, Canada*
- TP 309 **Measuring a Slice of the Exposome: Targeted GC-MS/MS Analysis of Persistent Organic Pollutants (POPs) in Small Volumes of Human Plasma;** Anthony Macherone<sup>1,2</sup>; Sarah Daniels<sup>3</sup>; Alex L. Maggitti<sup>4</sup>; Melissa Churley<sup>1</sup>; Matthew McMullin<sup>4</sup>; Martyn T. Smith<sup>3</sup>; <sup>1</sup>Agilent Technologies, Wilmington, DE; <sup>2</sup>Johns Hopkins School of Medicine, Baltimore, MD; <sup>3</sup>University of California, Berkeley, CA; <sup>4</sup>NMS Labs, Willow Grove, PA
- TP 310 **Fate of Anti-Inflammatory Drug Diclofenac in Municipal Wastewater Treatment Plant: Quantification using LDTD Coupled with Tandem Mass Spectrometry;** Linson Lonappan<sup>1</sup>; Rama Pulicharla<sup>1</sup>; Serge Auger<sup>2</sup>; Satinder K. Brar<sup>1</sup>; Mausam Verma<sup>3</sup>; Roa Y. Surampalli<sup>4</sup>; <sup>1</sup>INRS-ETE, Université du Québec, Québec, Canada; <sup>2</sup>Phytronix Technologies, Quebec, Canada; <sup>3</sup>CO2 Solutions Inc., Quebec, Canada; <sup>4</sup>University of Nebraska-Lincoln, Lincoln, NE
- TP 311 **Determination of leachables in Orally Inhaled and Nasal Drug Products (OINDP) by GCMS/MS;** Prashant Hase; Ankush Bhone; Durvesh Sawant; Dheeraj Handique; Sanket Chiplunkar; Ajit Datar; Jitendra Kelkar; Pratap Rasam; *Shimadzu Analytical India Pvt. Ltd., Mumbai, India*
- TP 312 **Comparative Quantitation of Calibration Methods in Surface Water Analysis Using Online Preconcentration with Orbitrap Mass Spectrometry;** Jaewon Choi<sup>1</sup>; Wonseok Choi<sup>1</sup>; Yun S. Kim<sup>1</sup>; Charles Yang<sup>2</sup>; Dipankar Ghosh<sup>2</sup>; <sup>1</sup>K-water, 200 Shintanjinro Daeduck, KOREA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- TP 313 **Atmospheric Pressure Ionization Coupled to Tandem Quadrupole Mass Spectrometry for the Analysis of Pyrethroids in Waste Water;** Adam Ladak<sup>1</sup>; Lauren Mullin<sup>3</sup>; Hernando Olivos<sup>1</sup>; Douglas Stevens<sup>2</sup>; <sup>1</sup>Waters, Beverly, MA; <sup>2</sup>Waters, Milford, MA; <sup>3</sup>MTM Research Centre, Örebro University, Örebro, Sweden
- TP 314 **Application of LC-MS/MS for the Improved Detection of Pesticides in Cannabis Samples;** Jared Russell<sup>1</sup>; Jeff Dahl<sup>2</sup>; Liling Fang<sup>1</sup>; Willard Bankert<sup>1</sup>; <sup>1</sup>Shimadzu Scientific Instruments, Pleasanton, CA; <sup>2</sup>Shimadzu, Columbia, MD
- TP 315 **Fast and sensitive analysis of drug residues in water using on line SPE-UHPLC-MS/MS with ultra-fast polarity switching;** Mikael LEVI<sup>1</sup>; Caroline DUFOUR<sup>2</sup>; Isabelle VECCHIOLI<sup>2</sup>; Stephane MOREAU<sup>3</sup>; <sup>1</sup>Shimadzu France, Noisiel, France; <sup>2</sup>CARSO-LSEHL, Lyon, France; <sup>3</sup>Shimadzu Europe GmbH, Duisburg, Germany
- TP 316 **Research and Identification of Veterinary Antibiotic Residues in Environmental and Biological Matrices using LC-HESI-HRMS;** Morgan Sollicie; Audrey Roy-Lachapelle; Sébastien Sauvé; *Université de Montréal, Montréal, Canada*
- TP 317 **Transformation of Antidepressant Pharmaceuticals During Chlorination Disinfection Processes in Wastewater Treatment;** Melissa M. Schultz; Derrick Marshall; Kent Nakamoto; *The College of Wooster, Wooster, OH*
- TP 318 **Screening and Quantitation of Micro Pollutants from Sewage Water in the Process of Bank Filtration Using UHPLC-HRMS;** Patricia van Baar<sup>1</sup>; Florian Wode<sup>1</sup>; Uwe Duennbier<sup>1</sup>; Maciej Bromirski<sup>2</sup>; Olaf Scheibner<sup>2</sup>; <sup>1</sup>Berliner Wasserbetriebe, Berlin, Germany; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany



- TP 319 **Highly Sensitive Detection of Pharmaceuticals and Personal Care Products (PPCPs) in Water Using Direct Injection**; Dan-Hui Dorothy Yang; Yanan Yang; *Agilent Technologies, Inc, Santa Clara, CA*
- TP 320 **Comparison of matrix effects in multi-residue pesticide analysis when using online SPE or direct injection in Liquid Chromatography-tandem Mass Spectrometry**; Sigrid Baumgarten<sup>1</sup>; Vincent Gohier<sup>2</sup>; Mikael Levi<sup>1</sup>; <sup>1</sup>*Shimadzu France, Noisiel, France*; <sup>2</sup>*Laboratoire Départemental d'Analyse de Corrèze, Tulle, France*
- TP 321 **Quantitative Analysis of Source Water PPCP by Offline SPE with Orbitrap MS and LC-Tandem MS**; Jaewon Choi<sup>1</sup>; Wonseok Choi<sup>1</sup>; Yun S. Kim<sup>1</sup>; Charles T. Yang<sup>2</sup>; Dipankar Ghosh<sup>2</sup>; <sup>1</sup>*Kwater, Daejeon, South Korea*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, California*
- TP 322 **Screening and Quantitation of 240 Pesticides in Difficult Food Matrices Using the Agilent 6545 QTOF Mass Spectrometer**; Dorothy Yang; Christian Klein; Crystal Cody; Huy Bui; *Agilent Technologies, Inc, Santa Clara, CA*
- TP 323 **Environmental Site Assessment using LC/MS/MS and GC/MS for Phenoxo Family of Pesticides: Data Comparison**; Vyacheslav N. Fishman; Ying Yang; *The Dow Chemical Company, Midland, MI*
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324-355**
- TP 324 **Simultaneous Determination of Allergens in Food Products Discovered to Validated Using Microfluidic Chip-Based Nano-Liquid Chromatography/Quadrupole Time Of Flight(Chip/Q-TOF) and Ultra High Performance Liquid Chromatography Ifunnel/Tandem Mass Spectrometry(iFunnel/QQQ)**; Wen-Yen Lee; Shan-An Chan; *Agilent, Taipei, Taiwan*
- TP 325 **High Sensitive Detection and Quantification of Synthetic PDE-5 Inhibitors Drugs and Analogues Adulterated in Health Supplements Using LC/MS/MS**; Zhe Sun; Jie Xing; Zhaoli Zhan; *Customer Support Centre, Singapore (Asia Pacific) Pte Ltd, 79 Science Park Drive, #02-01/08, Singapore 118264*
- TP 326 **Food Contact Material (FCM) Migration Study using HR-LCMS and Novel Software Database Suite**; Allan Brown<sup>1</sup>; Kate Comstock<sup>2</sup>; Ekong Bassy<sup>2</sup>; David Kage<sup>2</sup>; Daniel Quinn<sup>2</sup>; <sup>1</sup>*Scholle Packaging, Northlake, IL*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*
- TP 327 **Direct Detection of Chlorpyrifos in Honey by Neutral Desorption-Extractive Electrospray Ionization Mass Spectrometry**; Xingxing Liu<sup>1</sup>; Li-Ping Luo<sup>1</sup>; Xiaowei Fang<sup>2</sup>; Eric Handberg<sup>2</sup>; Huanwen Chen<sup>2</sup>; <sup>1</sup>*School of Life Sciences, Nanchang University, Nanchang, China*; <sup>2</sup>*East China Institute of Tech., Nanchang, China*
- TP 328 **Differentiating Rice Varieties by SPME-GC-MS and NMR Chemical Profiling**; Xinyi Wang; Peter B. Harrington; *Department of Chemistry and Biochemistry, Ohio U, Athens, OH*
- TP 329 **Atmospheric Pressure Ionization GC Coupled to Time of Flight Mass Spectrometry for the Analysis of Agriculture Residues in Food Safety**; Gordon Fujimoto<sup>1</sup>; Andrew Baker<sup>2</sup>; Adam Ladak<sup>1</sup>; Kerri Smith<sup>1</sup>; <sup>1</sup>*Waters Corporation, Beverly, MA*; <sup>2</sup>*Waters, Inc., Pleasanton, CA*
- TP 330 **LC-MS/MS Analysis of Perfluoroalkyl Acids in Environmental Samples, Food Packaging Material and Food – A Migration and Accumulation Study**; Andre Schreiber<sup>1</sup>; Liesl Krone<sup>2</sup>; KC Hyland<sup>3</sup>; Tom Biesenthal<sup>1</sup>; Tanya Gamble<sup>1</sup>; Chris Higgins<sup>4</sup>; <sup>1</sup>*SCIEX, Concord, Canada*; <sup>2</sup>*Granbury High School, Granbury, TX*; <sup>3</sup>*SCIEX, Redwood City, CA*; <sup>4</sup>*Colorado School of Mines, Golden, CO*
- TP 331 **Investigating the Impact of Frozen Storage on the Anthocyanin Content of American Elderberry Fruit Juice Using Mass Spectrometry**; Mitch Johnson<sup>1</sup>; Andrew Thomas<sup>2,3</sup>; C. Michael Greenleaf<sup>1,2</sup>; <sup>1</sup>*University of Missouri, Columbia, MO*; <sup>2</sup>*Center for Botanical Interaction Studies, MU, Columbia, MO*; <sup>3</sup>*Southwest Research Center, University of Missouri, Mt. Vernon, MO*
- TP 332 **Quantitative Determination of Seven Fluorescent Whitening Agents Migration of paper cups by High Performance Liquid Chromatography Tandem Mass Spectrometry**; ZhiFeng Du<sup>1</sup>; XinDong Guo<sup>2</sup>; JinFeng Huang<sup>2</sup>; LiJun Li<sup>3</sup>; WenHai Jin<sup>4</sup>; HuaFen Liu<sup>5</sup>; HuaiEn Zhu<sup>4</sup>; <sup>1</sup>*Sciex, GuangZhou, China*; <sup>2</sup>*National Centre for Quality Supervision, GuangZhou, China*; <sup>3</sup>*Sciex, BeiJing, BeiJing*; <sup>4</sup>*Sciex, ShangHai, China*; <sup>5</sup>*Sciex, America, America*
- TP 333 **HR-LCMS and GC-MS/MS Analyses of Non-Intentionally Added Substances and other Migrants from Plastic Food Contact Materials**; Ian Cooper<sup>1</sup>; Andrew Feilden<sup>2</sup>; Kate Comstock<sup>3</sup>; Cristian Cojocariu<sup>4</sup>; Paul Silcock<sup>4</sup>; <sup>1</sup>*Smithers Pira, Leatherhead, UK*; <sup>2</sup>*Smithers Rapra, Shrewsbury, UK*; <sup>3</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>4</sup>*Thermo Fisher Scientific, RunCorn, UK*
- TP 334 **Quantitative Analysis of Illegal Dyes in Eggs Using LC/MS/MS**; Rashi Kochhar; Shailendra Rane; Shruti Raju; Deepti Bhandarkar; Shailesh Damale; Ajit Datar; Jitendra Kelkar; Pratap Rasam; *Shimadzu Analytical (India) Pvt. Ltd., Mumbai, INDIA*
- TP 335 **Simultaneous Determination of 20 Polyfluoroalkane Substances in Dietary Milk by QuEChERS Combining with On-Line Interference Trapping LC-MS/MS**; Yucheng Yu<sup>1</sup>; Dunming Xu<sup>1</sup>; Meiling Lu<sup>2</sup>; Shan Zhou<sup>2</sup>; Yu Zhou<sup>1</sup>; <sup>1</sup>*Xiamen Entry-Exit Inspection and Quarantine Bureau, Xiamen, CN*; <sup>2</sup>*Agilent Technologies (China) Limited, Beijing, China*
- TP 336 **Puff by puff investigation of New Smoking Products such as e-cigarettes and 'Heat-Not-Burn' Devices Using Online Photoionization Mass Spectrometry**; Sven Ehler<sup>1</sup>; Andreas Walte<sup>2</sup>; Ralf Zimmermann<sup>1</sup>; <sup>1</sup>*University of Rostock, Rostock, Germany*; <sup>2</sup>*Photonion GmbH, Schwerin, Germany*
- TP 337 **Illegal Color Dyes in Food Matrix for Multi-Compounds Analysis with Agilent 6460QQQ and 6545Q-TOF**; Shao-Zhen Wang<sup>1</sup>; Yong Zhou<sup>2</sup>; Ping-Ya Wang<sup>2</sup>; Ai Chen<sup>2</sup>; Li Huang<sup>2</sup>; Jin-Lan Sun<sup>1</sup>; Heng-Tao Dong<sup>1</sup>; Chun-Ye Sun<sup>1</sup>; <sup>1</sup>*Agilent Technology, Inc., Shanghai, China*; <sup>2</sup>*Institute for Food and Drug Control, Zhoushan, China*
- TP 338 **Determination of Chemical Contaminants in Marine Fish by GCMS/MS using QuEChERS as an Extraction Method**; Ankush Bhone; Durvesh Sawant; Dheeraj Handique; Prashant Hase; Sanket Chiplunkar; Ajit Datar; Jitendra Kelkar; Pratap Rasam; *Shimadzu Analytical (India) Pvt. Ltd., Mumbai, INDIA*
- TP 339 **The Analysis of Chlorinated Dioxins, Difurans and Polychlorinated Biphenyls in Edible Oils**; Justin Blau; Greg Jeter; *Fluid Management Systems, Watertown, MA*
- TP 340 **The Analysis of Chlorinated Dioxins and Difurans in Pet Food**; Greg Jeter; Ryan Balgos; *Fluid Management Systems, Watertown, MA*
- TP 341 **Determination of Brominated Fatty Acids in Brominated Vegetable Oils and Commercial Beverages by UPLC-MS-MS**; Priyanka Chitranshi; Goncalo Gamboa Da Costa; *FDA/NCTR, Jefferson, AR*
- TP 342 **Analysis of Mercury in Grouper by ICP MS: An Evaluation of Mercury Levels in the Commercial Catch**; Marc E. Engel; *FDACS, Tallahassee, FL*
- TP 343 **Analysis of Mycotoxins Using LC-MS/MS and a QuEChERS Sample Preparation Approach**; Brian Kinsella; *UCT, Bristol, PA*
- TP 344 **Development of an Interface for the Analysis of Volatiles Using a Portable Mass Spectrometer**; Pilar Perez Hurtado<sup>1</sup>; Elliott Palmer<sup>1</sup>; Clive Aldcroft<sup>2</sup>; Hanna More<sup>2</sup>; Baker Andrew<sup>2</sup>; Mark Allen<sup>2</sup>; Jamey Jones<sup>2</sup>; Matthew Turner<sup>1</sup>; Jim Reynolds<sup>1</sup>; <sup>1</sup>*Loughborough University, Loughborough, UK*; <sup>2</sup>*Advion UK Ltd, Essex, UK*

- TP 345 **Analysis of 7 Plasticizers Released from Microwave-Treated Food Wraps Using GC-MS;** Matt S. Chang; Sheng Hsiung Yang; Jeremiah Y. Shen; Gaston J. Wu\*; *Department of Chemistry, NTNU, Taipei City, Taiwan (R.O.C.)*
- TP 346 **Low Level Quantitation of Steroids in Milk Using LC/MS/MS;** Durvesh Sawant; Rashi Kochhar; Shailendra Rane; Shruti Raju; Deepti Bhandarkar; Shailesh Damale; Ajit Datar; Jitendra Kelkar; Pratap Rasam; *Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*
- TP 347 **Rapid Authentication of Mixed Edible Oils by Matrix-assisted Laser Desorption/Ionization Mass Spectrometry;** Tsz-Tsun Ng; Pui-Kin So; Bo Zheng; Zhong-Ping Yao; *The Hong Kong Polytechnic University, Hong Kong, China*
- TP 348 **ICP-MS Method for the Determination of Boric Acid in Caviar;** Jung Bok Kim<sup>1</sup>; Jang So-Young<sup>1</sup>; kim Joo Taek<sup>1</sup>; Kim Myung Chul<sup>1</sup>; Lee Ok Hwan<sup>2</sup>; Shin Jae Wook<sup>1</sup>; <sup>1</sup>*Korea Advanced Food Research institute, Seocho-Gu, KOREA;* <sup>2</sup>*Kang-Won National University, Chuncheon, Korea*
- TP 349 **High Sensitivity Analysis of Diarrhetic Shellfish Poisoning (DSP) Toxins Using Liquid Chromatography Tandem Mass Spectrometry;** Manami Kobayashi<sup>1</sup>; Miho Kawashima<sup>2</sup>; Satoshi Yamaki<sup>1</sup>; Yoshihiro Hayakawa<sup>3</sup>; <sup>1</sup>*Shimadzu Corporation, Kanagawa, Japan;* <sup>2</sup>*Shimadzu Corporation, Tokyo, Japan;* <sup>3</sup>*Shimadzu Corporation, Kyoto, Japan*
- TP 350 **Determination of a Single Methodology for the Analysis and Quantitation of Multi-class Veterinary Drugs in Different Animal Matrices;** Ed George; Charles T. Yang; Dipankar Ghosh; Mary Blackburn; *Thermo Fisher Scientific, San Jose, CA*
- TP 351 **Accurate Multi-Mycotoxin Quantification in Feed Materials Using LC-MS/MS Methods and Isotopic or Structural Analog Dilution Strategies Revolutionize Mycotoxin Occurrence Understanding;** Alexandros Yiannikouris; Joshua Martinez; Steve Mobley; *Alltech Inc., Nicholasville, KY*
- TP 352 **Rapid Screening and Confirmation of PDE5 Inhibitors in Dietary Ingredients by DART-MS Ambient Ionization;** Robert Goguen; Julie Carbonello; Elizabeth Crawford; Brian D. Musselman; *IonSense, Inc., Saugus, MA*
- TP 353 **ELISA-based Screening for Alternative Nitrogenous Economic Adulterants in Milk Proteins;** Nicholas Cellar<sup>1</sup>; Michael Farrow<sup>1</sup>; Nicholas Baldauf<sup>2</sup>; Todime M. Reddy<sup>1</sup>; <sup>1</sup>*Abbott, Columbus, OH;* <sup>2</sup>*Advance Testing Laboratories, Cincinnati, OH*
- TP 354 **Study on Carbosulfan Metabolites in Vegetable by Ultra-High Performance Liquid Chromatography Tandem Quadrupole-Time Of Flight Mass Spectrometry;** Jianzhong Li; Tao Bo; *Agilent Technologies(China), Beijing, China*
- TP 355 **Quantitation of Chloramphenicol and Nitrofurantol Metabolites in Aquaculture Products Using Microwave-Assisted Derivatization, Automated Solid-Phase Extraction and LC-MS/MS;** Brian Veach; *Food and Drug Administration, Jefferson, AR*
- MICROORGANISMS: IDENTIFICATION AND CHARACTERIZATION 356-370**
- TP 356 **Simultaneous Identification of Multiple  $\beta$ -Lactamases in *Acinetobacter baumannii* using Liquid Chromatography-Tandem Mass Spectrometry;** Hein Trip<sup>1</sup>; Katrin Mende<sup>2</sup>; Joanna Majchrzykiewicz-Koehorst<sup>1</sup>; Norbert Sedee<sup>1</sup>; Albert Hulst<sup>1</sup>; Hugo-Jan Jansen<sup>3</sup>; Clinton Murray<sup>2</sup>; Armand Paauw<sup>1</sup>; <sup>1</sup>*CBRN Protection, TNO, Rijswijk, The Netherlands;* <sup>2</sup>*Department of Medicine, San Antonio Military Med, Fort Sam Houston, TX;* <sup>3</sup>*Expert Centre Force Health Protection, MoD, Doorn, The Netherlands*
- TP 357 **Rapid detection of Fluoroquinolone-Resistant *Escherichia coli* using Mass Spectrometry;** Tiphaine Cecchini<sup>1,2</sup>; Silpak Biswas<sup>3</sup>; Tanguy Fortin<sup>1,4</sup>; Marc Galimand<sup>3</sup>; Gilles Zambardi<sup>5</sup>; Xavier Lacoux<sup>1</sup>; Arnaud Salvador<sup>2</sup>; Gaspard Gervasi<sup>1</sup>; Jerome Lemoine<sup>2</sup>; Patrice Courvalin<sup>3</sup>; Jean-Philippe Charrier<sup>1</sup>; <sup>1</sup>*bioMerieux, Marcy L'Etoile, France;* <sup>2</sup>*ISA, Unit 5280 CNRS/UCBL-1, Villeurbanne, France;* <sup>3</sup>*Unité des Agents Antibactériens, Institut Pasteur, Paris, France;* <sup>4</sup>*Anaquant, Villeurbanne, France;* <sup>5</sup>*bioMerieux, La Balme-Les-Grottes, France*
- TP 358 **Label-Free Quantitation Reveals the Importance of Host Cell Arginine Uptake in *Francisella phagosomal* Escape and Ribosomal Protein Amounts;** Cerina Chhuon<sup>1,3</sup>; Elodie Ramond<sup>2,3</sup>; Gael Gesbert<sup>2,3</sup>; Ida Chiara Guerrera<sup>1,3</sup>; Marion Dupuis<sup>2,3</sup>; Mélanie Rigard<sup>4</sup>; Thomas Henry<sup>4</sup>; Monique Barel<sup>2,3</sup>; Alain Charbit<sup>2,3</sup>; <sup>1</sup>*Proteomics Platform Necker, Paris, France;* <sup>2</sup>*INSERM U1151, Institut Necker-Enfants Malades, Paris, France;* <sup>3</sup>*Université Paris Descartes, Sorbonne Paris Cité, Paris, France;* <sup>4</sup>*Centre International de Recherche en Infectiologie, Lyon, France*
- TP 359 **Application of Mass Spectrometry as a Confirmatory Tool for *Campylobacter* Species Identification;** Philippe Raymond<sup>1</sup>; Rebecca A Guy<sup>2</sup>; Maxime Gosselin-Théberge<sup>2</sup>; Sylvianne Paul<sup>1</sup>; <sup>1</sup>*Canadian Food Inspection Agency, St-Hyacinthe, Canada;* <sup>2</sup>*Public Health Agency of Canada, St-Hyacinthe, Canada*
- TP 360 **Enhanced Detection and Identification of Shiga toxin 1 and 2 from Pathogenic Bacteria by MALDI-TOF-TOF-MS/MS-PSD and Top-Down Proteomic Analysis;** Clifton K. Fagerquist; William J. Zaragoza; USDA/ARS, Albany, CA
- TP 361 **Top-Down Analysis of Penicillin Binding Protein 2a from Methicillin Resistant *Staphylococcus Aureus*;** Jason Neil<sup>1</sup>; Helene Cardasis<sup>1</sup>; Ping Yip<sup>1</sup>; Vikrant Gohil<sup>1</sup>; Alexander Cherkassky<sup>1</sup>; James Stephenson<sup>2</sup>; <sup>1</sup>*Thermo Fisher Scientific, Cambridge, MA;* <sup>2</sup>*Thermo Fisher Scientific, Raleigh, NC*
- TP 362 **MALDI-TOF-MS for the Differentiation of Strains of Cyanobacteria by Their Secondary Metabolites Profile;** João Luiz Bronzel Junior; Milena Luizete; Ana C. Codo; Humberto Milagre; *UNESP - Univ Estadual Paulista - Institute of Chem, Araraquara, Brazil*
- TP 363 **MALDI-TOF-MS Identification and Characterization of Fungal Pathogens Associated with Cereal Grains;** Kumaran Sivagnanam<sup>1</sup>; Helene Perreault<sup>2</sup>; Tom Gräfenhan<sup>1</sup>; <sup>1</sup>*Canadian Grain Commission, Winnipeg, Canada;* <sup>2</sup>*University of Manitoba, Winnipeg, Canada*
- TP 364 **Monitoring Chemical Communication and Chemotypical Differentiation in *Pseudomonas aeruginosa* Microbial Communities Using Confocal Raman Microscopy and Secondary Ion Mass Spectrometry;** Sage Dunham<sup>1</sup>; Nameera Baig<sup>2</sup>; Nydia Morales-Soto<sup>2</sup>; Eric Lanni<sup>1</sup>; Joshua ShROUT<sup>2</sup>; Paul Bohn<sup>2</sup>; Jonathan Sweedler<sup>1</sup>; <sup>1</sup>*University of Illinois at Urbana Champaign, Urbana, IL;* <sup>2</sup>*University of Notre Dame, Notre Dame, IN*
- TP 365 **MALDI Biotyper Analysis of Microorganisms Present in Saliva of Chronic Kidney Disease Individuals and their Association with Periodontal Disease;** Levy Alves<sup>1</sup>; Taciana Couto<sup>1</sup>; Ana Ciamponi<sup>1</sup>; Marcelo Fava<sup>2</sup>; Meriellen Dias<sup>3</sup>; Maria Anita Mendes<sup>3</sup>; <sup>1</sup>*Faculdade de Odontologia - São Paulo University, Sao Paulo, Brazil;* <sup>2</sup>*Faculdade de Medicina - São Paulo University, São Paulo, Brazil;* <sup>3</sup>*Engenharia Química - Poli - São Paulo University, São Paulo, Brazil*
- TP 366 **Metaproteomic Analysis of Human Cervical-Vaginal Fluid in Residual Pap Tests: Insights into the Cervical Microbiome;** Somaieh Afiuni-Zadeh<sup>1</sup>; Pratik Jagtap<sup>2</sup>; Timothy Griffin<sup>1</sup>; Marnie Peterson<sup>1</sup>; Amy Skubitz<sup>1</sup>; <sup>1</sup>*University of Minnesota, Minneapolis, MN;* <sup>2</sup>*Center for Mass Spectrometry and Proteomics, UMN, St. Paul, MN*



- TP 367 **Glycoproteins with Fucosylated O-glycans are Associated with the Nuclear Membrane of Toxoplasma gondii**; [Edwin M Motari](#)<sup>1</sup>; Giulia Bandini<sup>1</sup>; Catherine E. Costello<sup>2</sup>; Samuelson John<sup>1</sup>; <sup>1</sup>*Boston University School of Dental Medicine, Boston, MA*; <sup>2</sup>*Boston University School of Medicine, Boston, MA*
- TP 368 **Identification of Food Borne Microorganism by MALDI-TOF MS**; Miyoung Ha<sup>2</sup>; Eun Kyoung Choi<sup>1</sup>; Jun Young Yang<sup>1</sup>; Jooyeon Oh<sup>1</sup>; [Sung Hun Kim](#)<sup>1</sup>; Yangsun Kim<sup>1</sup>; Kyu H Park<sup>1</sup>; <sup>1</sup>*ASTA, Suwon-Si, South Korea*; <sup>2</sup>*Nonghyup Food Safety Research Institute, Seoul, South Korea*
- TP 369 **Analysis of Intact Cowpea Mosaic Virus by MALDI TOF Mass Spectrometry Incorporating Superconducting Tunnel Junction Cryodetection**; Logan Plath<sup>1</sup>; Jonathan Feldman<sup>1</sup>; Anna Czapar<sup>2</sup>; Nicole Steinmetz<sup>2</sup>; [Mark E. Bier](#)<sup>1</sup>; <sup>1</sup>*Carnegie Mellon University, Pittsburgh, PA*; <sup>2</sup>*Case Western Reserve University, Cleveland, OH*
- TP 370 **Dental Plaque meta-omics for Diagnosis of Oral and Systemic Disease**; [Timothy W. Rhoads](#)<sup>1</sup>; Nicholas W. Kwiecien<sup>1</sup>; Anna E. Merrill<sup>1</sup>; Michael S. Westphall<sup>1</sup>; Sanjay Shukla<sup>2</sup>; Amit Acharya<sup>2</sup>; Joshua J. Coon<sup>1</sup>; <sup>1</sup>*University of Wisconsin, Madison, WI*; <sup>2</sup>*Marshfield Clinic Research Foundation, Marshfield, WI*
- H/D EXCHANGE: PROTEIN STRUCTURE/FUNCTION  
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- TP 371 **Structural Dynamics of the 180 kDa HIV-1 Initiation Complex Investigated Using Hydrogen-Deuterium Exchange Mass Spectrometry**; [Devrishi Goswami](#)<sup>1</sup>; Steve Tuske<sup>2</sup>; Bruce D. Pascal<sup>3</sup>; Joseph D. Bauman<sup>2</sup>; Disha Patel<sup>2</sup>; Eddy Arnold<sup>2</sup>; Patrick R. Griffin<sup>1</sup>; <sup>1</sup>*The Scripps Research Institute, Jupiter, FL*; <sup>2</sup>*Center for Advanced Biotechnology and Medicine, De, Piscataway, NJ*; <sup>3</sup>*Informatics core, The Scripps Research Institute, Jupiter, FL*
- TP 372 **Revealing the Architecture of Protein Complexes by an Orthogonal Approach Combining HDXMS, CXMS and Disulphide Trapping**; [Kunhong Xiao](#)<sup>1</sup>; Sheng Li<sup>2</sup>; <sup>1</sup>*Duke University Medical Cent, Durham, NC*; <sup>2</sup>*University of California at San Diego, La Jolla, CA*
- TP 373 **Electrostatics-Driven Conformational Dynamics of Cellobiose Dehydrogenase Probed by Structural Mass Spectrometry**; [Alan Kadek](#)<sup>1,2</sup>; Roland Ludwig<sup>3</sup>; Petr Halada<sup>1</sup>; Petr Man<sup>1,2</sup>; <sup>1</sup>*Institute of Microbiology CAS, Prague, Czech Republic*; <sup>2</sup>*Faculty of Science, Charles University in Prague, Prague, Czech Republic*; <sup>3</sup>*U. of Natural Resources and Applied Life Sciences, Vienna, Austria*
- TP 374 **Identifying Dynamical Profiles Associated with Toxicity of Reginoid X Receptor Agonist by use of Hydrogen Deuterium Exchange Mass Spectrometry**; [Emily Cowart](#); Amanda Proper; Matthew Renfrow; Donald Muccio; *University of Alabama at Birmingham, Birmingham, AL*
- TP 375
- TP 376 **Combining HDX-MS, Raman and SAXS Provides Low Resolution Models of a Large Intrinsically Disordered Protein, which Folds upon Ligand Binding**; [Darragh Patrick O'Brien](#)<sup>1</sup>; Véronique Hourdel<sup>1</sup>; Belen Hernandez<sup>2</sup>; Patrice Vachette<sup>3</sup>; Ana-Cristina Sotomayor-Pérez<sup>1</sup>; Mahmoud Ghomi<sup>2</sup>; Julia Chamot-Rooke<sup>1</sup>; Daniel Ladant<sup>1</sup>; Dominique Durand<sup>3</sup>; Sébastien Brier<sup>1</sup>; Alexandre Chenal<sup>1</sup>; <sup>1</sup>*Institut Pasteur, Paris, France*; <sup>2</sup>*Université Paris 13, Paris, France*; <sup>3</sup>*Université Paris-Sud, Paris, France*
- TP 377 **Mapping Calmodulin-Induced Conformational Changes during Activation of Neuronal Nitric Oxide Synthase by H/D Exchange Mass Spectrometry**; [Eric Underbakke](#)<sup>1</sup>; Brian Smith<sup>2</sup>; <sup>1</sup>*Iowa State University, Ames, IA*; <sup>2</sup>*Medical College of Wisconsin, Milwaukee, WI*
- TP 378 **Bottom-up HX-MS2 Analysis Applied to 620kDa of Unique Sequence**; [Morgan Hoepfner](#); Yaping Yu; Susan Lees-Miller; David Schriemer; *University of Calgary, Calgary, Canada*
- TP 379 **Structural Changes during Dimerization of the Type IV Pilin from Pseudomonas aeruginosa strain K122-4 Measured by Time-Resolved Hydrogen-Deuterium Exchange**; [Cristina Lento](#); Gerald Audette; Derek Wilson; *York University, Toronto, Canada*
- TP 380 **Probing Conformational Changes Occurring at the Calmodulin Interface upon Adenylate Cyclase Binding Using HDX-MS and Statistical Analysis**; Darragh Patrick O'Brien; Stevonn Volant; Véronique Hourdel; Maryline Davi; Marie-Agnes Dillies; Daniel Ladant; Julia Chamot-Rooke; Alexandre Chenal; [Sébastien Brier](#); *Institut Pasteur, Paris, France*
- TP 381 **Changes in Structural Conformation of the C-terminal Domain of Human La Protein upon RNA binding by Hydrogen/Deuterium Exchange Mass Spectrometry**; [Kerene Brown](#); Mark Bayfield; Derek Wilson; *York University, Toronto, ON*
- TP 382 **Curli Amyloid Protein Aggregation Studies by HDX Mass Spectrometry**; [Hanliu Wang](#); Qin Shu; Don L. Rempel; Carl Frieden; Michael L. Gross; *Washington University, St Louis, MO*
- TP 383 **Dynamic Changes during Acid-Induced Activation of Influenza Hemagglutinin**; [Natalie Garcia](#); Miklos Guttman; Jamie Ebner; Alexander Mileant; Lee Kelly; *University of Washington, Seattle, WA*
- TP 384 **Correlating Dynamic Conformational Sampling to Enzyme Catalysis: A Millisecond Timescale Hydrogen/Deuterium Exchange Mass Spectrometry Approach**; [Peter Liuni](#); Derek Wilson; *Department of Chemistry, York University, Toronto, ON*
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- TP 385 **Top-Down Quantitative Proteomics Reveals Novel Mechanistic Insights in Acute Myocardial Infarction**; [Zachery Gregorich](#); Ying Peng; Ying-Hua Chang; Lichen Xiu; Santosh Valeja; Ying Ge; *UW Madison, Madison, WI*
- TP 386 **Automated Glyco-Proteform Network Analysis (PNA) on Top-Down MS (TDMS) Datasets**; Steven M. Patrie<sup>1,2</sup>; John Corbett<sup>1,2</sup>; Daniel Plymire<sup>1</sup>; <sup>1</sup>*University of Texas Southwestern Medical Center, Dallas, TX*; <sup>2</sup>*University of Texas at Dallas, Richardson, TX*
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- TP 388 **Novel Strategies to Address the Challenges in Top-Down Mass Spectrometry-Based Proteomics**; [Ying Ge](#); Zachery Gregorich; Leekyoung Hwang; Lichen Xiu; Santosh G Valeja; Ying-Hua Chang; Wenxuan Cai; Ying Peng; Song Jin; *University of Wisconsin-Madison, Madison, WI*
- TP 389 **pTop 1.0: a Highly Efficient Search Engine for Intact Protein Identification**; [Lan Luo](#); Rui-Xiang Sun; Long Wu; Hao Chi; Chao Liu; Si-Min He; *Institute of Computing Technology, CAS, Beijing, China*
- TP 390 **Improving Top-Down Proteomics Sequence Coverage through Complementary Fragmentation Approaches**; [Si Wu](#)<sup>1</sup>; Da Meng<sup>3</sup>; Li Cao<sup>4</sup>; Ljiljana Pasa-Tolic<sup>3</sup>; Xiaowen Liu<sup>2</sup>; <sup>1</sup>*University of Oklahoma, Norman, OK*; <sup>2</sup>*IUPUI, Indianapolis, IN*; <sup>3</sup>*Pacific NW Nat'l Lab, Richland, WA*; <sup>4</sup>*vaccine production program laboratory, Gaithersburg, MD*
- TP 391 **A Searchable Public Repository for Archiving Known Proteoforms**; [Ryan Fellers](#); Richard Leduc; Bryan Early; Joseph Greer; Paul Thomas; Neil L. Kelleher; *Northwestern University, Evanston, IL*

- TP 392 **Top-down MS Analysis of Membrane-bound Light Harvesting Complex 2 from Purple Bacteria;** Yue Lu; Hao Zhang; Michael L. Gross; Robert E. Blankenship; *Washington University, St Louis, MO*
- TP 393 **Optimizing Top Down Analysis of Proteins on an Orbitrap Fusion Tribrid Mass Spectrometer;** Seema Sharma<sup>1</sup>; Parag Mallick<sup>2</sup>; Tanya Stoyanova<sup>3</sup>; Christopher Mullen<sup>1</sup>; Chad Weisbrod<sup>1</sup>; Jesse Canterbury<sup>1</sup>; David Horn<sup>1</sup>; Vlad Zabrouskov<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*Stanford University, Stanford, CA*; <sup>3</sup>*University of California Los Angeles, Los Angeles, CA*
- TP 394 **Characterization of Tropomyosin Proteoforms in Skeletal Muscle by Top-Down Mass Spectrometry;** Yutong Jin; Ying Peng; Yi-Chen Chen; Timothy Hacker; Ying Ge; *University of Wisconsin-Madison, Madison, WI*
- TP 395 **Optimization of LC/MS Intact /Top-Down Protein Analysis on an Orbitrap Fusion Mass Spectrometer;** Rosa Viner; Seema Sharma; Jesse D. Canterbury; David Horn; Vlad Zabrouskov; *Thermo Fisher Scientific, San Jose, CA*
- TP 396 **In-Line Separation by Capillary Electrophoresis prior to Analysis by Top-Down Mass Spectrometry Enables Sensitive Characterization of Protein Complexes;** Xuemei Han<sup>1</sup>; Aaron Aslanian<sup>1</sup>; Bryan Fonslow<sup>1,2</sup>; Daniel McClatchy<sup>1</sup>; Beth Graczyk<sup>3</sup>; Trisha N. Davis<sup>3</sup>; John Yates<sup>1</sup>; <sup>1</sup>*The Scripps Research Institute, La Jolla, CA*; <sup>2</sup>*AB SCIEX, San Diego, CA*; <sup>3</sup>*University of Washington, Seattle, WA*
- TP 397 **Exploring Depth and Breadth of a Protein Complex Mixture with Top-Down Data-Independent Acquisition Using an Orbitrap Fusion Tribrid Mass Spectrometer;** Aaron Bailey; David Horn; Seema Sharma; Romain Huguet; Vlad Zabrouskov; *Thermo Fisher Scientific, San Jose, CA*
- TP 398 **Performance Evaluation of the Q Exactive™ HF Hybrid Quadrupole-Orbitrap Mass Spectrometer for High-Throughput Top-Down Proteomics;** Eugen Damoc<sup>1</sup>; Ping Yip<sup>2</sup>; Leena Valmu<sup>3</sup>; Alexander Cherkassky<sup>2</sup>; Bernard Delanghe<sup>1</sup>; Eduard Denisov<sup>1</sup>; Oksana Gvozdyak<sup>2</sup>; Helene Cardasis<sup>2</sup>; Jason Neil<sup>2</sup>; Alexander Makarov<sup>1</sup>; Jim Stephenson<sup>2</sup>; <sup>1</sup>*Thermo Fisher Scientific, Bremen, Germany*; <sup>2</sup>*Thermo Fisher Scientific, Cambridge, MA*; <sup>3</sup>*Thermo Fisher Scientific, Vantaa, Finland*
- TP 399 **Automated Multi-Dimensional Top-Down Clinical Proteomics Platform for High Sensitivity and Quantitative Proteoform Analysis on Individual Patient Cerebrospinal Fluid;** John Corbett<sup>1,2</sup>; Daniel Plymire<sup>1</sup>; Steven Patrie<sup>1,2</sup>; <sup>1</sup>*University of Texas Southwestern Medical Center, Dallas, TX*; <sup>2</sup>*University of Texas at Dallas, Richardson, TX*
- TP 400 **Fractionation by Size Exclusion Chromatography of Proteins for Top-Down Analysis;** Lucia Geis-Asteggiante<sup>1</sup>; Suzanne Ostrand-Rosenberg<sup>2</sup>; Catherine Fenselau<sup>1</sup>; <sup>1</sup>*University of Maryland, College Park, MD - Maryland*; <sup>2</sup>*University of Maryland Baltimore County, Baltimore, MD*
- TP 401 **A Novel Three Dimensional Liquid Chromatography Platform for Top-down Proteomics;** Lichen Xiu; Santosh Valeja; Zachery Gregorich; Huseyin Guner; Song Jin; Ying Ge; *University of Wisconsin-Madison, Madison, WI*
- TP 402 **Top-Down, High-Throughput Proteomics of Thermo-Stable Allergens Using Complementary MS/MS Fragmentation Strategies;** Monica Carrera<sup>1</sup>; Daniel Lopez Ferrer<sup>2</sup>; Chad Weisbrod<sup>2</sup>; Romain Huguet<sup>2</sup>; Jose Manuel Gallardo<sup>1</sup>; Jae C. Schwartz<sup>2</sup>; Andreas Huhmer<sup>2</sup>; <sup>1</sup>*CSIC, Vigo, SPAIN*; <sup>2</sup>*ThermoFisher Scientific, San Jose, CA*
- TP 403 **Identification of Proteoforms from Yeast Lysate Using Measurements of Intact Mass and Lysine Count;** Brian L. Frey; Michael R. Shortreed; Mark Scalf; Rachel A. Knoener; Anthony J. Cesnik; Lloyd M. Smith; *University of Wisconsin, Madison, WI*
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- TP 404 **Evaluation of Different Alternatives to In-Gel-Digestion of Proteins;** Moritz Neupärtl; Marion Bäumlisberger; Philip Hölltaler; Michael Karas; *Goethe University, Frankfurt Am Main, Germany*
- TP 405 **Improving Protein LC/MS Analysis;** Barry Boyes<sup>1,2</sup>; Stephanie Schuster<sup>1</sup>; Joseph Kirkland<sup>1</sup>; Benjamin Libert<sup>1</sup>; Brian Wagner<sup>1</sup>; Joseph Destefano<sup>1</sup>; <sup>1</sup>*Advanced Materials Technology Inc., Wilmington, DE*; <sup>2</sup>*University of Georgia, Athens, GA*
- TP 406 **Integration of Electrochemistry with Ultra-Performance Liquid Chromatography/Mass Spectrometry (UPLC/MS);** Yi Cai<sup>1</sup>; Qiuling Zheng<sup>1</sup>; Yong Liu<sup>2</sup>; Roy Helmy<sup>2</sup>; Joseph A. Loo<sup>3</sup>; Hao Chen<sup>1</sup>; <sup>1</sup>*Ohio University, Athens, OH*; <sup>2</sup>*Merck Research Laboratories, Merck & Co., Inc., Rahway, NJ*; <sup>3</sup>*University of California-Los Angeles, Los Angeles, CA*
- TP 407 **Mass Spectrometry of Collagen Preserved in Archaeological Specimens Including Human Bones;** Shunsuke Fukakusa<sup>1</sup>; Kazuki Kawahara<sup>2</sup>; Mehdi Moini<sup>3</sup>; Takashi Nakazawa<sup>1</sup>; <sup>1</sup>*Nara Women's University, Nara, Japan*; <sup>2</sup>*Osaka University, Suita, Osaka*; <sup>3</sup>*George Washington University, Washington DC*
- TP 408 **General Protein Analysis Using in-source CID and SEC Chromatography;** Dale Schoener; John Cremin; Michael Buonarati; *Intertek Pharmaceutical Services, El Dorado Hills, CA*
- TP 409 **A Knowledge-Based Approach to Developing a Mass Spectrometry Method for Detection of Gluten in "Free-From" Foods;** Sophie Bromilow<sup>1</sup>; Lee A Gethings<sup>2</sup>; Prof. Peter Shewry<sup>3</sup>; Michael Buckley<sup>1</sup>; Michael Bromley<sup>4</sup>; Phil Johnson<sup>1</sup>; Prof. Clare Mills<sup>1</sup>; <sup>1</sup>*University of Manchester, Manchester, UK*; <sup>2</sup>*Waters, Manchester, N/A*; <sup>3</sup>*Rothamsted Research, Harpenden, UK*; <sup>4</sup>*Synergy Health, Swindon, UK*
- TP 410 **Small Molecule Inhibition of Beta-2 Microglobulin Amyloid Formation Studied by Mass Spectrometry;** Tyler Marcinko; Patrick Kiefer; William Warren; Kate Daborowski; Richard Vachet; *University of Massachusetts, Amherst, MA*
- TP 411 **Use of MALDI-MS in the Detection of Non-Covalent Amyloid  $\beta$  Oligomers;** Jasmine S.-H. Wang<sup>1,2</sup>; Kristina Jurcic<sup>1</sup>; Shawn N. Whitehead<sup>2</sup>; Ken K.-C. Yeung<sup>1</sup>; <sup>1</sup>*Department of Chemistry and Biochemistry, London, ON*; <sup>2</sup>*Department of Anatomy and Cell Biology, London, ON*
- TP 412 **Development of a Combined Workflow to Study the Relationship Between Cysteine Accessibility in the Active Site and Protein Aggregation;** Natalya Atlasevich; Pilsoo Kang; Jianmei Kochling; *Genzyme, Framingham, MA*
- TP 413 **Protein Characterization Involved in Mussel Byssal Threads Biogenesis by 2D-LC-MS/MS;** Maxime Sansoucy<sup>1</sup>; Cynthia Caron<sup>1</sup>; Réjean Tremblay<sup>2</sup>; Isabelle Marcotte<sup>1</sup>; Lekha Sleno<sup>1</sup>; <sup>1</sup>*UQAM, Montreal, Canada*; <sup>2</sup>*UQAR-ISMER, Rimouski, Canada*
- TP 414 **Characterizing High Molecular Weight Glutentin Subunits in Canadian Wheat Varieties Using ESI-MS on Intact Protein;** Ray Bacala; Dave Hatcher; *Canadian Grain Commission, Winnipeg, Canada*
- TP 415 **Mass spectrometric characterization of Coenzyme Q biosynthesis;** Arne Ulbrich; Catherine E. Minogue; Jon A. Stefely; Danielle C. Lohman; Andrew G. Reidenbach; Michael S. Westphall; David J. Pagliarini; Joshua J. Coon; *University of Wisconsin, Madison, WI*
- TP 416 **Correlation between Protein Concentrations and Recovery in SDS PAGE;** David Fabacher; Ute Bahr; Michael Karas; *Goethe University, Frankfurt am Main, Germany*
- TP 417 **Venomics of *Nephilingis cruentata* Spider by Data Dependent and Data Independent Acquisition Methods in Mass Spectrometry;** Rafael Lomazi<sup>1</sup>; Thiago Abreu<sup>1</sup>;



- Josias Pagotto<sup>1</sup>; Eduardo Kitano<sup>2</sup>; Solange Serrano<sup>2</sup>; Pedro Silva Jr.<sup>2</sup>; Alexandre Keiji Tashima<sup>1</sup>; <sup>1</sup>*EPM/Universidade Federal de São Paulo, São Paulo, Brazil*; <sup>2</sup>*LETA/ Instituto Butantan, Sao Paulo, Sao Paulo*
- TP 418 **On-target Tryptic Digest and MALDI-MS Analysis of Reproduction Proteins from *Pieridae* Butterflies**; Måns Ekelöf; Maria Kihon Rokhas; Johan Jacksén; Åsa Emmer; *KTH Royal Institute of Technology, Stockholm, SWEDEN*
- TP 419 **Trypsin modified membrane reactors for controlled and limited proteolysis followed by mass spectrometry**; Wenjing Ning; Jinlan Dong; Merlin Bruening; *Michigan State University, East Lansing, MI*
- TP 420 **Investigating the Cellular Interactions of BIRB796 Analogs Using a Novel Chloroalkane Capture Tag**; Marjeta Urh<sup>1</sup>; Rachel Friedman Ohana<sup>1</sup>; Robin Hurst<sup>1</sup>; Thomas Kirkland<sup>2</sup>; Sergiy Levin<sup>2</sup>; Michael Ford<sup>3</sup>; Richard Jones<sup>3</sup>; Keith Wood<sup>1</sup>; <sup>1</sup>*Promega, Madison, WI*; <sup>2</sup>*Promega Biosciences LLC, San Luis Obispo, CA*; <sup>3</sup>*MS Bioworks LLC, Ann Arbor, MI*
- TP 421 **Characterization of a Novel NUDIX Hydrolase Using Limited Proteolysis, Bottom-Up, and Middle-Down Mass Spectrometry**; Lauren R Devine; Robert O'Meally; Andres H de la Peña; Sandra B Gabelli; Robert N Cole; *Johns Hopkins, Baltimore, MD*
- TP 422 **Protein Fractionation by Subcellular Location to Enhance Proteomic Coverage of Cultured Cells**; Haiyan Wu; Ryan Bomgardner; Kay Opperman; John C. Rogers; Barb Kaboord; *Thermo Fisher Scientific, Rockford, IL*
- TP 423 **Integrating Mass Spectrometry and Structural Biology Techniques to Investigate a Novel Bacterial Ferritin-Like Protein**; Sally Vanden-Hehir<sup>1</sup>; Didi He<sup>1</sup>; Sophie Harvey<sup>2</sup>; C. Logan Mackay<sup>1</sup>; Jon Marles-Wright<sup>1</sup>; David J Clarke<sup>1</sup>; <sup>1</sup>*University of Edinburgh, Edinburgh, UK*; <sup>2</sup>*Ohio State University, Columbus, OH*
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- TP 424 **Characterizing Time-Course GaINAc-T Reactions at the Molecular Level Using nanoLC-MS with Relative Quantification Yields New Insight into Clustered O-Glycosylation**; Tyler Stewart<sup>1</sup>; Kazuo Takahashi<sup>2</sup>; Milan Raska<sup>3</sup>; Qi Bian<sup>1</sup>; Zhi-qiang Huang<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>*Fujita Health University, Toyoake, Japan*; <sup>3</sup>*University of Palacky, Olomouc, Czech Republic*
- TP 425 **The Use of MRM Methods for Glycan Discovery and Extensive Characterization of Site-Specific Glycosylation**; Muchena J. Kailemia; Carlito Lebrilla; *University of California, Davis, CA*
- TP 426 **Investigation of Detergent and Detergent Free Sample Preparations for Membrane Proteomics/ Glycoproteomics of Breast Cancer Cells with different Clinicopathological Features**; Yu Zhang; Rui Zhu; Shiyue Zhou; Yehia Mechref; *Texas Tech University, Lubbock, TX*
- TP 427 **Tissue-Specific Protein Glycosylation and the Detection of Sialic Acid Variants at the Glycopeptide Level**; Katalin F. Medzihradsky; Krista Kaasik; Robert J. Chalkley; *UCSF, San Francisco, CA*
- TP 428 **Developing Methods for Analyzing N-Glycans Released from Low-Abundant Human Plasma Proteins**; Cheylene Tanimoto; Sarah Totten; Sharon Pitteri; *Stanford University School of Medicine, Palo Alto, CA*
- TP 429 **SugarCone: a Software of Automatic Glycopeptide Sequencing by Y1 and peptide ion of N- and O-linked Glycopeptide**; Chen-Hung Chen; Hsin-Yu Hsieh; Jung-Lee Lin; Chung-Hsuan Chen; *Academia Sinica, Taipei, Taiwan*
- TP 430 **Unraveling the Cell Surface Glycoproteome**; Rebecca Sosa; Yanyan Qu; William Alley; *University of Texas at San Antonio, San Antonio, TX*
- TP 431 **Comprehensive Monitoring of Glycopeptides Alternation in Cancer Patients by Multiple Reaction Monitoring and Precursor Ion Scan**; Petra Dabebna<sup>2</sup>; Petr Novak<sup>1,2</sup>; Radek Kucera<sup>3</sup>; Ondrej Topolcan<sup>3</sup>; Miloslav Sanda<sup>4</sup>; Radoslav Goldman<sup>4</sup>; Petr Pompach<sup>1,2</sup>; <sup>1</sup>*Institute of Microbiology, Prague, Czech Republic*; <sup>2</sup>*Charles University, Prague, Czech Republic*; <sup>3</sup>*Faculty Hospital in Pilsen, Pilsen, Czech Republic*; <sup>4</sup>*Georgetown University, Washington, DC, DC*
- TP 432 **Glycomic Profiling of Biofluids and Exosomes by MALDI-FTICR**; Huarong Xu; Thomas Powers; Roper Stephen; Richard R Drake; *Medical University of South Carolina, Charleston, SC*
- TP 433 **Defining a Glycosylation Site of Human PSA Prompted by Missense Mutation by LC-MS/MS**; Ehwang Song<sup>1</sup>; Yunli Hu<sup>1</sup>; Chuan-Yih Yu<sup>2</sup>; Haixu Tang<sup>2</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>*Texas Tech University, Lubbock, TX*; <sup>2</sup>*Indiana University, Bloomington, IN*
- TP 434 **Mass Spectrometry Analysis of Glycoproteins of the Sulfate Reducer *Archaeoglobus fulgidus***; Deborah R. Leon<sup>1</sup>; Cheng Lin<sup>1</sup>; Nancy Leymarie<sup>2</sup>; Rachel R. Ogorzalek Loo<sup>3</sup>; Joseph A. Loo<sup>3</sup>; Robert P Gunsalus<sup>3</sup>; Catherine E. Costello<sup>2</sup>; <sup>1</sup>*Boston University School of Medicine, Boston, MA*; <sup>2</sup>*Boston University School of Medicine, Boston, MA*; <sup>3</sup>*UCLA, Los Angeles, CA*
- TP 435 **The Characterization of Glycosylated Neuropeptides from the Lobster, *Homarus americanus***; Henry E. Pratt<sup>1</sup>; Patsy S. Dickinson<sup>1</sup>; Andrew E. Christie<sup>2</sup>; Elizabeth A. Stemmler<sup>1</sup>; <sup>1</sup>*Bowdoin College, Brunswick, ME*; <sup>2</sup>*University of Hawaii at Manoa, Honolulu, HI*
- TP 436 **A Method for Simultaneous Analysis of N-Linked Glycans, Glycosites, and Site-Specific Glycan Heterogeneity for Comprehensive Characterization of Glycoproteins**; Shisheng Sun<sup>2</sup>; Punit Shah<sup>1</sup>; Shadi Toghi Eshghi<sup>1</sup>; Weiming Yang<sup>1</sup>; Namita Trikannad<sup>1</sup>; Shuang Yang<sup>1</sup>; Lijun Chen<sup>1</sup>; Paul Aiyetan<sup>1</sup>; Naser Uddin Hoti<sup>1</sup>; Daniel W. Chan<sup>1</sup>; Hui Zhang<sup>1</sup>; <sup>1</sup>*John Hopkins Dept. of Pathology, Baltimore, MD*; <sup>2</sup>*Johns Hopkins University, Baltimore, Maryland*
- TP 437 **Site-specific modulation of surface glycoprotein sialylation upon short time stimulation of HeLa cells**; María Ibáñez-Vea; Lylia Drici; Veit Schwämmle; Pernille Lassen; Giuseppe Palmisano; Lene Jakobsen; Martin R. Larsen; *University of Southern Denmark, Odense, Denmark*
- TP 438 **HILIC and ERLIC Enrichment of Glycopeptides Derived From Breast and Brain Cancer Cells**; Lauren Zacharias; Ehwang Song; Alyssa Hartmann; Rui Zhu; Parvin Mirzaei; Yehia Mechref; *Texas Tech University, Lubbock, TX*
- TP 439 **An Optimized Method for the Deglycosylation, Enrichment, and Derivatization of N-linked Glycans from Proximal Biofluids**; Crystal Daniels<sup>1,2</sup>; Jana Rocker<sup>1,2</sup>; Lewis Pannell<sup>1,2</sup>; <sup>1</sup>*University of South Alabama, Mobile, AL*; <sup>2</sup>*Mitchell Cancer Institute, Mobile, AL*
- TP 440 **Comprehensive and High Throughput Quantitative Site-Specific N-Linked Glycosylation Analysis of Recombinant Glycoproteins**; Xiaoying Jin<sup>1</sup>; Dongyu Liu<sup>2</sup>; Lin Liu<sup>1</sup>; Joanne Cotton<sup>1</sup>; Clarence Wang<sup>2</sup>; Xiaokui Kate Zhang<sup>1</sup>; <sup>1</sup>*Sanofi Biotherapeutics, Framingham, MA*; <sup>2</sup>*Genzyme, Framingham, MA*
- TP 441 **A Pipeline Employing Native MS to Analyze Glycoproteins and Glycoprotein Complexes from Endogenous Samples**; Rafael D. Melani<sup>1,2</sup>; Luis H. F. do Vale<sup>3</sup>; Owen Skinner<sup>1</sup>; Luca Fornelli<sup>1</sup>; Marcelo V. Sousa<sup>3</sup>; Gilberto Domont<sup>2</sup>; Philip Compton<sup>1</sup>; Neil L. Kelleher<sup>1</sup>; <sup>1</sup>*Northwestern University, Evanston, IL*; <sup>2</sup>*Univ Federal Do Rio De Janeiro, Rio De Janeiro, Brazil*; <sup>3</sup>*Universidade de Brasília, Brasília, Brazil*

- TP 442 **Integrated N-Glycoproteomics-Based Assessment of Equivalence between Induced Pluripotent Stem Cells and Embryonic Stem Cells**; Putty-Reddy Sudhir<sup>1</sup>; Madireddy Pavana Kumari<sup>1</sup>; Wei-Ting Hsu<sup>2</sup>; Hung-Chih Kuo<sup>2</sup>; Chung-Hsuan Chen<sup>1</sup>; <sup>1</sup>GRC, Academia Sinica, Taipei, Taiwan; <sup>2</sup>ICOB, Academia Sinica, Taipei, Taiwan
- TP 443 **Identification of N-Glycans Using an Accurate Mass and Retention Time Database Yield Oligosaccharides Variations in Individual Serum**; Ting Song<sup>1</sup>; Stephen Madden<sup>2</sup>; Carlito Lebrilla<sup>1</sup>; <sup>1</sup>University of California Davis, Davis, CA; <sup>2</sup>Agilent Technologies, Inc., Santa Clara, CA
- TP 444 **Quantification of Glycopeptides from Human Prostate Specific Antigen using Multiple Reaction Monitoring**; Masaki Kurogouchi<sup>1</sup>; Toshio Nakamura<sup>1</sup>; Yusuke Inohana<sup>2</sup>; Ichiro Hirano<sup>2</sup>; Junko Amano<sup>1</sup>; <sup>1</sup>the noguchi institute, Tokyo, Japan; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan
- TP 445 **Analysis of N-Linked Glycopeptides Derived from Human Liver Tissues by LC-MS/MS**; Minkun Wang<sup>1,2</sup>; Cristina Di Poto<sup>1</sup>; Ehwang Song<sup>3</sup>; Rui Zhu<sup>3</sup>; Yehia Mechref<sup>3</sup>; Habtom Ressom<sup>1</sup>; <sup>1</sup>Georgetown University, Lombardi Cancer Center, Washington, DC; <sup>2</sup>Virginia Tech, Arlington, VA; <sup>3</sup>Texas Tech University, Lubbock, TX
- TP 446 **In-Depth Analysis of Site-Specific N-Glycosylated alpha 1 Acid Glycoprotein and Vitronectin from Human Plasma**; Juyeon Lee<sup>1</sup>; Heeyoun Hwang<sup>1</sup>; Gun Wook Park<sup>1,2</sup>; Hyun Kyoung Lee<sup>1,2</sup>; Jin Youn Kim<sup>1</sup>; Jong Shin Yoo<sup>1,2</sup>; <sup>1</sup>Korea Basic Science Institute, Chungbuk, South Korea; <sup>2</sup>Graduate School of Analytical Science and Technol, Daejeon, South Korea
- TP 447 **Studying the Kinetics of N-glycan Release by PNGase F with MRM Quantitation of the Glycopeptides from Human Serum Glycoproteins**; Yining Huang; Adam Kramer; Ron Orlando; University of Georgia, Athens, GA
- TP 448 **Integrative Omics Analysis to Reveal the Molecular Biological Mechanism of Breast Cancer Brain Metastasis**; Wenjing Peng; Rui Zhu; Shiyue Zhou; Ehwang Song; Parvin Mirzaei; Lauren Zacharias; Yunli Hu; Kameswara Rao Kottapalli; Yehia Mechref; Texas Tech University, Lubbock, TX
- PROTEINS: PHOSPHOPROTEINS**  
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- TP 449 **A Global Survey of Protein Phosphorylation Reveals its Extensive Regulatory Network in Rat Fetal Neural Stem Cells**; Shuxin Wang<sup>1</sup>; Xuyang Zhao<sup>2</sup>; Qingsong Wang<sup>1</sup>; Jianguo Ji<sup>1</sup>; <sup>1</sup>Peking University, Beijing, China; <sup>2</sup>Peking University Health Science Center, Beijing, China
- TP 450 **Phosphoproteomics of Human Immunodeficiency Virus-1**; Pratikumar Rathod<sup>1,2</sup>; Hsin-Pin Ho<sup>1,2</sup>; Xu Yu<sup>3</sup>; Dr. Mathias Lichterfeld<sup>3,4</sup>; Dr. Emmanuel Chang<sup>1,2</sup>; <sup>1</sup>York College- City University of New York, Jamaica, NY; <sup>2</sup>Graduate Center- City University of New York, New York, NY; <sup>3</sup>Ragon Institute of MGH, MIT and Harvard, Cambridge, MA; <sup>4</sup>Infectious Disease Division- MGH, Boston, MA
- TP 451 **Using Phosphoproteomics to Reveal the ATM Dependent Mediators in the Late Phase of Replication Stress**; Stephanie Munk; Luis I. Toledo; Louise von Stechow; Jiri Lukas; Jesper V. Olsen; NNF CPR, University of Copenhagen, Copenhagen, DENMARK
- TP 452 **Label-free Quantitative Determination of LPS- and TNF $\alpha$ -induced Phosphorylation dynamics on IRAK4 involved in the Host Immune Response**; Li Wang; Harsha P. Gunawardena; Xian Chen; University of North Carolina at Chapel Hill, Chapel Hill, NC
- TP 453 **Phospho-Signaling Pathways and Cross-Talk in SKBR3 Breast Cancer Cells**; Fumio Ikenishi; Iuliana Lazar; Virginia Tech, Blacksburg, VA
- TP 454 **Microfluidic Reactor for Fast Proteolytic Digestion and Enrichment in Phosphopeptides**; Jingren Deng; Iulia M. Lazar; Department of Biological Sciences, Virginia Tech, Blacksburg, VA
- TP 455 **A Scoring Model for Phosphopeptide Site Localization and its Impact on the Question of Whether to Use MSA**; Juliana Fischer<sup>2</sup>; Marlon dos Santos<sup>2</sup>; Fabricio Marchini<sup>1</sup>; Valmir Barbosa<sup>3</sup>; Paulo Carvalho<sup>2</sup>; Nilson Zanchin<sup>2</sup>; <sup>1</sup>Carlos Chagas Institute, Fiocruz , Pr, Curitiba, Brazil; <sup>2</sup>Laboratory for Proteomics and Protein Engineering, Curitiba, Brazil; <sup>3</sup>Federal University of Rio de Janeiro, Rio de Janeiro, Brazil
- TP 456 **Functionalized Multivalent Nanoparticles for Top-down Phosphoproteomics**; Leekyoung Hwang; Bifan Chen; Serife Ayaz-Guner; Tania Guardado; Ying Peng; Zachery Gregorich; Song Jin; Ying Ge; University of Wisconsin-Madison, Madison, WI
- TP 457 **Automated Phosphopeptide Spectral Library Searching for Fast and Confident Site Localisation**; Veronika Suni<sup>1</sup>; Susumu Imanishi<sup>1</sup>; Garry Corthals<sup>1,2</sup>; <sup>1</sup>Turku Centre for Biotechnology, Turku, Finland; <sup>2</sup>University of Amsterdam, Amsterdam, The Netherlands
- TP 458 **Identification of Phosphorylation Sites in Marine Microbes**; Noelle Held; Mak Saito; Woods Hole Oceanographic Institution, Woods Hole, Massachusetts
- TP 459 **A Sensitive Assay to Measure Total Protein Phosphorylation Level in Complex Protein Samples**; Li Pan; Linna Wang; Chuan-Chih Hsu; Jiazhen Zhang; Anton Iliuk; Weiguo Andy Tao; Purdue University, West Lafayette, IN
- TP 460 **Identification of Post-Translational Modifications on HEXIM1 that Regulate the Activation of P-TEFb and HIV Proviral Reactivation**; Benlian Wang<sup>1</sup>; Uri Mbonye<sup>2</sup>; Giridharan Gokulrangan<sup>3</sup>; Jonathan Karn<sup>2</sup>; Mark R. Chance<sup>1</sup>; <sup>1</sup>Center for Proteomics and Bioinformatics, CWRU, Cleveland, OH; <sup>2</sup>Dept. of Molecular Biology and Microbiology, CWRU, Cleveland, OH; <sup>3</sup>PDM Department, Pfizer WRD, Andover, MA
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- TP 465 **Comparative LC-MS Profiling of the Cell Surface of NSCLC Cell Lines Bearing Oncogenic K-RAS Mutations**; [Xiaoying Ye](#); Robert Stephens; Gordon Whiteley; Josip Blonder; *Leidos Biomedical Research, Inc., Fredrick Nationa, Frederick, MD*
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- TP 468 **Applying Native nESI-IMS-MS and FPOP with LC-MS to the Study of Membrane Proteins**; [Tom G Watkinson](#); Antonio N Calabrese; Sheena E Radford; Alison E Ashcroft; *University of Leeds, Leeds, UK*
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- TP 470 **Effect of Surfactant, Solvents and Digestion Conditions on Digestion Efficiency of Drug Transporter Proteins by Trypsin**; [Buyun Chen](#); Liling Liu; Alan Deng; Brian Dean; Emile Plise; Laurent Salphati; Yuan Chen; Xiaorong Liang; *Genentech, South San Francisco, CA*
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- TP 472 **Activation and Oligomerization of Bax Studied by Ion Mobility Mass Spectrometry**; [Jeroen Van Dyck](#)<sup>1</sup>; Albert Konijnenberg<sup>1</sup>; Frank Sobott<sup>1,2</sup>; <sup>1</sup>University of Antwerp BAMS group, Antwerp, Belgium; <sup>2</sup>Center for Proteomics, Antwerp, Belgium
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- TP 474 **Mass Spectrometric Analysis of Surface Exposed Regions in the Hexadecameric Phosphorylase Kinase Complex**; [Mary Ashley Rimmer](#); Antonio Artigues; Owen W Nadeau; Maria T Villar; Victor Vasquez-Montes; Gerald M Carlson; *University of Kansas Medical Center, Kansas City, KS*
- TP 475 **Analysis of Affinity-Isolated Endogenous Protein Complexes by Native Mass Spectrometry Using an Exactive Plus EMR Instrument**; [Paul Dominic B. Olinares](#); Julio C. Padovan; Brian T. Chait; *The Rockefeller University, New York, NY*
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- TP 477 **Discovery of Lipid Acquisition Mechanism of *Plasmodium vivax* in Liver Stage by Interactome Technique**; [Supachai Topanurak](#)<sup>1</sup>; Peerut Chienwichai<sup>1</sup>; Wang Nguitragoon<sup>1,2</sup>; Jetsumon Prachumsri<sup>2</sup>; <sup>1</sup>Faculty of Tropical Medicine, Mahidol University, Bangkok, Thailand; <sup>2</sup>Mahidol Vivax Research Unit, Mahidol University, Bangkok, Thailand
- TP 478 **CSNAP – the 9th Subunit of the COP9 Signalosome Complex**; [Gili Ben-Nissan](#); Maria Gabriela Fuzesi-Levi; Rozen Shelly; Michal Sharon; *Weizmann Institute of Science, Rehovot, Israel*
- TP 479 **Analysis of the Apoptosis Signal-Regulating Kinase Signalosome Dynamics by Targeted Mass Spectrometry**; [Joel Federspiel](#); Simona Codreanu; Daniel Liebler; *Vanderbilt University School of Medicine, Nashville, TN*
- TP 480 **Structural Proteomics Analysis of the tau-Protein – Microtubule**; Karl Makepeace<sup>1</sup>; Evgeniy Petrochenko<sup>1</sup>; [Nicole Sessler](#)<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada; <sup>2</sup>Dept. of Biochem. & Microbiol., Univ. of Victoria, Victoria, BC, Canada
- TP 481 **Crosslinking Analysis of Fibrin Polymerization**; [Karl Makepeace](#)<sup>1</sup>; Evgeniy Petrochenko<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada; <sup>2</sup>Dept. of Biochem. & Microbiol., Univ. of Victoria, Victoria, BC, Canada
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- TP 484 **A Study of the MEK1 Interactome Dynamics by Affinity Purification-Mass Spectrometry Reveals Novel Interactors**; [Laura Herring](#)<sup>1</sup>; Kyle Grant<sup>2</sup>; Kevin Blackburn<sup>1</sup>; Jason Haugh<sup>1</sup>; Michael Goshe<sup>1</sup>; <sup>1</sup>North Carolina State University, Raleigh, NC; <sup>2</sup>UNC-Chapel Hill, Chapel Hill, NC
- TP 485 **Proteomic Analysis of the Essential Mitotic Activator Bora and its Regulation in the Human Cell Cycle**; [Andrew Grasseti](#); Mark Adamo; Scott Rusin; Arminja Kettenbach; Scott Gerber; *Dartmouth Medical School, Hanover, NH*
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- TP 487 **Affinity Proteomics Establishes NIMA-Related Kinases as Regulators of Cytokinesis through Control of Microtubule Motor Localization**; [Sierra Cullati](#); Scott Gerber; *Geisel School of Medicine at Dartmouth, Lebanon, NH*
- TP 488 **Discovering a New Subunit for an Old Complex**; Shelly Rozen; Maria Fuzesi-Levi; Gili Ben-Nissan Ben-Nissan; [Michal Sharon](#); *Weizmann Institute of Science, Rehovot, Israel*
- TP 489 **Filtering and Scoring of Results from AP-MS Experiments by Spectral Counts, Label-Free Quantitation and Enrichment Factor**; [Roman Mylonas](#)<sup>1,2</sup>; Patrice Waridel<sup>2</sup>; Manfredo Quadroni<sup>2</sup>; <sup>1</sup>Vital-IT Group - Swiss Institute of Bioinformatics, Lausanne, Switzerland; <sup>2</sup>CIG - University of Lausanne, Lausanne, Switzerland
- TP 490 **New Developments for the CRAPome Resource for Scoring AP-MS Protein Interaction Data**; [Dattatreya Mellacheruvu](#)<sup>1</sup>; Zachary Wright<sup>1</sup>; Anne-Claude Gingras<sup>2</sup>; Alexey Nesvizhskii<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>Samuel Lunenfeld Research Institute, Mount Sinai H, Toronto, ON
- TP 491 **Identification of Yeast Mediator Complex Interacting Proteins by 15N Metabolic Labeling**; [Henriette Uthe](#); Jens T. Vanselow; Andreas Schlosser; *Wuerzburg, Germany*

TP 492 **Improving Detection Efficiency of Large, Complex Ions Generated Under Native Conditions Using an Electrically Biased Pixelated Detector**; Tiffany Porta<sup>1,2</sup>; Andrey Dyachenko<sup>3</sup>; Shane R. Ellis<sup>1,2</sup>; Gert B. Eijkel<sup>1</sup>; Bob Hommersom<sup>1</sup>; Jerre van der Horst<sup>4</sup>; Dmitry Byelov<sup>5</sup>; Dirk-Jan Spaanderman<sup>2</sup>; Ronald Buijs<sup>2</sup>; Frans Giskes<sup>1</sup>; Albert J.R. Heck<sup>3</sup>; Ron M.A. Heeren<sup>1</sup>; <sup>1</sup>M4I Institute - Maastricht University, Maastricht, The Netherlands; <sup>2</sup>FOM Institute AMOLF, Amsterdam, The Netherlands; <sup>3</sup>Utrecht University, Utrecht, The Netherlands; <sup>4</sup>MS Vision, Almere, The Netherlands; <sup>5</sup>Omics2Image, Amsterdam, The Netherlands

TP 493 **Quantitative Measurement of the Protein Complex Landscape of Murine Tissues Using PCP-SILAC**; Nichollas E. Scott; Duncan Ferguson; Marjan Farahbod; Joerg Gsponer; Paul Pavlidis; Leonard J Foster; University of British Columbia, Vancouver, Canada

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TP 496 **Conformational Differences in Monoclonal Antibody Dimers Revealed by Hydrogen/Deuterium Exchange Mass Spectrometry**; Jun Zhang; Christopher Woods; Mei Han; Feng He; Michael Treuheit; Amgen, Inc, Seattle, WA

TP 497 **Multiple Reaction Monitoring (MRM)-Based Quantitation of Oxidation During Hydroxyl Radical Protein Footprinting for Pharmaceutical Protein Conformation Analysis**; Franklin E. Leach III<sup>1</sup>; Peter J. Todd<sup>1</sup>; Ron Orlando<sup>2</sup>; Joshua S. Sharp<sup>2</sup>; <sup>1</sup>Photochem Technologies, Athens, GA; <sup>2</sup>University of Georgia, Athens, GA

TP 498 **Characterization of IgG and IgM Monoclonal Antibodies by Superconducting Tunnel Junction Cryodetection MALDI TOF Mass Spectrometry**; Logan Plath; Jonathan Feldman; David Sipe; Mark E. Bier; Carnegie Mellon University, Pittsburgh, PA

TP 499 **Analytical Characterization of Therapeutic Monoclonal Antibodies in Cynomolgus Monkey Serum by Immunopurification and Mass Spectrometry**; Rosalynn Molden; Haibo Qiu; Ning Li; Thomas Daly; Regeneron Pharmaceuticals, Tarrytown, NY

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TP 503 **High Throughput Peptide Mapping with the Vanquish UHPLC and Q Exactive HF**; Martin Samonig<sup>1</sup>; Remco Swart<sup>1</sup>; Kai Scheffler<sup>2</sup>; Jonathan L. Josephs<sup>3</sup>; <sup>1</sup>Thermo Fisher Scientific, Germering, Germany; <sup>2</sup>Thermo Fisher Scientific, Dreieich, Germany; <sup>3</sup>Thermo Scientific, West Windsor, NJ

TP 504 **Comprehensive Characterization of Site-specific Engineered Antibody Drug Conjugate by Orbitrap Mass Spectrometer**; Hongxia (Jessica) Wang<sup>1</sup>; Terry Zhang<sup>1</sup>; Brian J. Agnew<sup>2</sup>; Rosa Viner<sup>1</sup>; Jonathan Josephs<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific, Eugene, OR

TP 505 **Intact Mass Analysis for Glycan Profiling of a Recombinant Therapeutic Protein Directly from Harvest Cell Culture**; Yunqiu (Rachel) Chen; Li Zang; Biogen Idec, Cambridge, MA

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TP 507 **Expression and Characterization of a Trastuzumab-Interferon Fusion Protein in Nicotiana benthamiana Plant to include in vitro Assay Results**; Earl L. White<sup>1</sup>; Lindsay Bennett<sup>1</sup>; Brian Berquist<sup>1</sup>; Iqbal Grewal<sup>3</sup>; Sanjay Khare<sup>3</sup>; Vally Kommineni<sup>1</sup>; Sylvain Marcel<sup>1</sup>; Ryan Murry<sup>2</sup>; Ranjith Munigunti<sup>1</sup>; Raj Sachdev<sup>3</sup>; Don Wilkerson<sup>1</sup>; Isaac Wong<sup>1</sup>; Barry Holtz<sup>1</sup>; <sup>1</sup>Caliber Biotherapeutics, LLC, Bryan, TX; <sup>2</sup>G-CON Manufacturing, Inc., College Station, TX; <sup>3</sup>ImmunGene, Inc., Camarillo, CA

TP 508 **Characterization of an IgG-Cleaving Protease from Streptococcus equi with Improved Activity Against Mouse IgGs**; Chris Hosfield<sup>1</sup>; Philip Compton<sup>2</sup>; Luca Fornelli<sup>2</sup>; Paul Thomas<sup>2</sup>; Neil L. Kelleher<sup>2</sup>; Michael Rosenblatt<sup>1</sup>; Marjeta Urh<sup>1</sup>; <sup>1</sup>Promega Corp, Madison, WI; <sup>2</sup>Northwestern University, Evanston, IL

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TP 510 **A Novel Data-Directed Approach for Comprehensive Disulfide Bond Mapping in Biotherapeutic Proteins**; Stephane Houel; Scott Geromanos; Steve Ciavarini; Weibin Chen; Waters Corp, Milford, MA

TP 511 **Monitoring Disulfide Bond Scrambling-An Enzyme Digestion pH Study**; Song Klapoetke; Michael J. Nold; KBI, Durham, NC

TP 512 **Mass Spectrometry Based Characterization of Multiple Critical Quality Attribute of Recombinant Human Collagen VII (rC7)**; Sheng Gu; Matthew Traylor; Craig Kaftan; Donald Gillies; Nicole Resendes; Bruce Tangarone; Shire, Lexington, MA

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TP 515 **An Ion-Current-Based, 44-plex Investigation of Influenza A Virus-Infected Mouse Lungs Revealed Altered Integrity of Lung Microvascular Barriers**; Shichen Shen<sup>1</sup>; Jun Li<sup>1</sup>; Xiaomeng Shen<sup>1</sup>; Andrew Ng<sup>1</sup>; Chengjian Tu<sup>1</sup>; Sina Ghaemmaghami<sup>2</sup>; Hulin Wu<sup>2</sup>; Martin Zand<sup>2</sup>; Jun Qu<sup>1</sup>; <sup>1</sup>SUNY at Buffalo, Buffalo, NY; <sup>2</sup>University of Rochester, Rochester, NY



- TP 516 **Application of High Sensitivity LC-MS/MS for Autoimmune Antigen Discovery in Antibiotic-refractory Lyme Arthritis or Rheumatoid Arthritis;** Qi Wang<sup>1</sup>; Elise E. Drouin<sup>2</sup>; Chunxiang Yao<sup>1</sup>; Jiyang Zhang<sup>3</sup>; Yu Huang<sup>1</sup>; Allen C. Steere<sup>2</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>*Boston University School of Medicine, Boston, MA*; <sup>2</sup>*Harvard Medical School, Boston, MA*; <sup>3</sup>*National University of Defense Technology, Changsha, Hunan Province, China*
- TP 517 **The Proteome of *Aedes aegypti* Legs from Female versus Male Mosquitoes;** Francine Perler; Colleen McClung; Ashley Luck; Cristian I. Ruse; *New England BioLabs, Ipswich, MA*
- TP 518 **Differential Protein Expression by Pathogenic *Leptospira* in Response to Mammalian Host Signals;** Jarlath Nally<sup>1</sup>; Stephen Hyland<sup>2</sup>; Andre Grassmann<sup>3</sup>; Melissa Caimano<sup>4</sup>; Kjell Sergeant<sup>5</sup>; Jenny Renaut<sup>6</sup>; <sup>1</sup>*NADC/USDA, Ames, IA*; <sup>2</sup>*University College Dublin, Dublin, Ireland*; <sup>3</sup>*Universidade Federal de Pelotas, Pelotas, Brazil*; <sup>4</sup>*University of Connecticut, Farmington, CT*; <sup>5</sup>*Luxembourg Institute of Science and Technology, Belvaux, Luxembourg*
- TP 519 **Protein Profiling of Three Distinct *Chlamydia trachomatis* Growth Forms;** Ole Østergaard; Anja Olsen; Peter Lawætz Andersen; Frank Follmann; Niels Henrik Helweg Heegaard; Ida Rosenkrands; *Statens Serum Institut, Copenhagen, Denmark*
- TP 520 **Investigation of Redox Control in *Chlamydia* Infection by Novel Chemical Tools and Mass Spectrometry;** Hanzhi Wu; Rosine Dushime; Xiaofei Chen; Nelmi O. Devarie-Baez; Cristina M. Furdui; Allen W. Tsang; *Wake Forest School of Medicine, Winston-Salem, NC*
- TP 521 **Quantitative and Structural Interaction Network of Nosocomial Pathogenesis;** Devin Schweppe; Arti Navare; Xia Wu; Larry Gallagher; Colin Manoil; James Bruce; *University of Washington, Seattle, WA*
- TP 522 **Novel inhibitor-Based Photoaffinity Labeling and MALDI Mass Spectrometry for Identification of Anti-Malarial Drug Targets.;** David Wood; Michael Prinsen; Megh Singh; Christopher Eickhoff; Francis Sverdrup; Marvin Meyers; *Saint Louis University, St. Louis, MO*
- TP 523 **Thioridazine Alters the Cell Envelope Permeability of *Mycobacterium tuberculosis*;** Jeroen De Keijzer<sup>1</sup>; Petra de Haas<sup>2</sup>; Arnoud de Ru<sup>1</sup>; Evy Heerkens<sup>2</sup>; Leonard Amaral<sup>3</sup>; Dick van Soolingen<sup>2</sup>; Peter van Veelen<sup>1</sup>; <sup>1</sup>*Leiden University Medical Centre, Leiden, the Netherlands*; <sup>2</sup>*National Institute for Public Health (RIVM), Bilthoven, the Netherlands*; <sup>3</sup>*Universidade Nova de Lisboa, Lisbon, Portugal*
- TP 524 **Membrane Proteome Characterization of Phenotypically Diverse *Pseudomonas aeruginosa* Cystic Fibrosis Isolates Reveals Adaptation to Host Lungs;** Karthik Shantharam Kamath<sup>1</sup>; Dana Pascovici<sup>2</sup>; Apurv Goel<sup>2</sup>; Anahit Penesyan<sup>1</sup>; Vignesh Venkatakrishnan<sup>1</sup>; Ian T Paulsen<sup>1</sup>; Nicolle H Packer<sup>1</sup>; Mark P Molloy<sup>1,2</sup>; <sup>1</sup>*Macquarie University, Sydney, Australia*; <sup>2</sup>*Australian Proteome Analysis Facility, Sydney, Australia*
- TP 525 ***Mycoplasma synoviae* Infection Induced Proteomic Changes In Chicken Serum;** Balamurugan Packialakshmi<sup>1</sup>; Rohana Liyanage<sup>1</sup>; Vijay Durairaj<sup>2</sup>; Jackson O Lay, Jr. <sup>1</sup>; Naola Ferguson-Noel<sup>2</sup>; Narayan Rath<sup>3</sup>; <sup>1</sup>*University of Arkansas, Fayetteville, AR*; <sup>2</sup>*The University of Georgia, Athens, GA*; <sup>3</sup>*PPPSRU, USDA-ARS, Fayetteville, AR*
- TP 526 **Molecular Anatomy of *Streptococcus Pyogenes* in Human Blood Plasma Using Absolute Quantification and Targeted Mass Spectrometry.;** Kristoffer Sjöholm; Lotta Happonen; Johan Malmström; *Lund University, Lund, Sweden*
- TP 527 **Succinylome Analysis Reveals the Involvement of Lysine Succinylation in Metabolism in Pathogenic *Mycobacterium tuberculosis* H37Rv;** Mingkun Yang<sup>2</sup>; Zhongyi Cheng<sup>1</sup>; Jing Gu<sup>2</sup>; Lijun Bi<sup>2</sup>; Feng Ge<sup>2</sup>; <sup>1</sup>*PTM Biolabs, Inc, Hangzhou, China*; <sup>2</sup>*Chinese Academy of Sciences, Wuhan, CN*
- TP 528 **Dynamic Regulation of Histone Deacetylase 5 (HDAC5) during HIV-1 Infection;** Amanda Guise<sup>1</sup>; Yang Luo<sup>2</sup>; Mark Muesing<sup>2</sup>; Ileana M. Cristea<sup>1</sup>; <sup>1</sup>*Princeton University, Princeton, NJ*; <sup>2</sup>*Aaron Diamond AIDS Research Center, New York, NY*
- TP 529 **The Epstein-Barr Virus Protein Kinase BGLF4 Integrates DNA Damage Response and Mitotic Phosphorylation Signaling to Promote Virus Replication;** Renfeng Li<sup>1</sup>; Raja Sekhar Nirujogi<sup>2,3</sup>; Sneha Pinto<sup>2,3</sup>; Gangling Liao<sup>2</sup>; Harsha Gowda<sup>3</sup>; Tai-Chung Huang<sup>2</sup>; Patrick Shaw<sup>2</sup>; Xinyan Wu<sup>2</sup>; Akhilesh Pandey<sup>2,3</sup>; S. Diane Hayward<sup>2</sup>; <sup>1</sup>*Virginia Commonwealth University, Richmond, VA*; <sup>2</sup>*Johns Hopkins University, Baltimore, MD*; <sup>3</sup>*Institute of Bioinformatics, Bangalore, India*

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- TP 530 **Single Cell Proteome Profiling Using Highly Sensitive LC-MS System and In-Capillary Sample Preparation Method;** Masaki Wakabayashi<sup>1</sup>; Jordan Aerts<sup>2</sup>; Elena Romanova<sup>2</sup>; Stanislav Rubakhin<sup>2</sup>; Yasushi Ishihama<sup>1</sup>; Jonathan Sweedler<sup>2</sup>; <sup>1</sup>*Kyoto University, Kyoto, Japan*; <sup>2</sup>*University of Illinois, Urbana, IL*
- TP 531 **Quantitatively Profiling Dynamic Proinsulin Processing by LC-MS;** Dongwan Cheng; Junjie Hou; Fuquan Yang; Tao Xu; *Institute of Biophysics, CAS, Beijing, China*
- TP 532 **Advancing Untargeted Proteomics to Single Cells for the 16-cell *Xenopus* Embryo using  $\mu$ CE-ESI-MS/MS;** Camille Lombard; Sally, A. Moody; Peter Nemes; *George Washington University, Washington, DC*
- TP 533 **MassAnalyzer as an Informatics Tool for Proteomics;** Zhongqi Zhang; Da Ren; Gang Xiao; Pavel Bondarenko; *Amgen, Inc., Thousand Oaks, CA*
- TP 534 **Fluorescence Complementation Mass Spectrometry (FCMS) for Identifying Direct Upstream Kinases;** Lingfei Zeng<sup>1</sup>; Wen-Hong Wang<sup>1</sup>; Robert Geahlen<sup>1</sup>; Chang-Deng Hu<sup>1</sup>; Andy Tao<sup>2</sup>; <sup>1</sup>*Department of MCMP, Purdue University, West Lafayette, IN*; <sup>2</sup>*Department of Biochemistry, Purdue University, West Lafayette, Indiana*
- TP 535 **Population Proteome Investigation of Pathogenicity and Persistence of *Pseudomonas aeruginosa* in Cystic Fibrosis Patient Airways;** Xia Wu; Benjamin Staudinger; Jayanthi Garudathri; Katherine Hisert; Colin Manoil; Pradeep Singh; James Bruce; *University of Washington, Seattle, WA*
- TP 536 **Absolute Quantitation of Non-Standard Amino Acids in Proteins Guiding the Evolution of Orthogonal Translation Systems;** Hans Rudolf Aerni<sup>1,2</sup>; Miriam Amiram<sup>2,3</sup>; Svetlana Rogulina<sup>1,2</sup>; Faren J. Isaacs<sup>2,3</sup>; Jesse Rinehart<sup>1,2</sup>; <sup>1</sup>*Cellular & Molecular Physiology, New Haven, CT*; <sup>2</sup>*Systems Biology Institute, West Haven, CT*; <sup>3</sup>*Molecular, Cellular and Developmental Biology, New Haven, CT*
- TP 537 **Discovering the Peptide Variants by Targeted Proteomics-Bioinformatics Pipeline;** Jerry C.D. Chen; *Chang Gung University, Taoyuan City, Taiwan (R.O.C)*
- TP 538 **In-Depth Melanoma Immunopeptidome for Anti-Tumor Immunotherapies;** Michal Bassani-Sternberg<sup>1</sup>; Eva Bräunlein<sup>2</sup>; Richard Klar<sup>2</sup>; Pavel Sinitcyn<sup>1</sup>; Julia Slotta-Huspenina<sup>3</sup>; Angelika Werner<sup>4</sup>; Rüdiger Hein Rüdiger<sup>5</sup>; Christian Peschel<sup>2</sup>; Dirk H. Busch<sup>6</sup>; Juergen Cox<sup>1</sup>; Angela M. Krackhardt<sup>2</sup>; Matthias Mann<sup>1</sup>; <sup>1</sup>*Max Planck Institute of Biochemistry, Martinsried, DE*; <sup>2</sup>*Medizinische Klinik III, Klinikum rechts der Isar, Munich, DE*; <sup>3</sup>*Institut für Allgemeine Pathologie und Pathologisch, Munich, DE*; <sup>4</sup>*Institute of Surgery, Klinikum rechts der Isar, Te, Munich, DE*; <sup>5</sup>*Department of Dermatology and Allergology, Technic, Munich, DE*; <sup>6</sup>*Institut für Medizinische Mikrobiologie, Immunologie, Munich, DE*

- TP 539 **A Universal Method for Peptide Identification;** Shannon Eliuk; Nina Soltero; Philip M Remes; Michael W. Senko; Vlad Zabrouskov; *Thermo Fisher Scientific, San Jose, CA*
- TP 540 **Enhancing Electrospray Response in Proteomics through Chemical Additives – Better Alternatives to DMSO;** Peng Yu; Hannes Hahne; Bernhard Kuster; *Technische Universität München, Freising, Germany*
- TP 541 **A New Probabilistic Score for the Chemical Cross-Linking Tandem Mass Spectrometry Data Analysis;** Mihir Jaiswal<sup>1,2</sup>; Boris Zybaylov<sup>2</sup>; <sup>1</sup>*University of Arkansas at Little Rock, University, Little Rock, AR*; <sup>2</sup>*University of Arkansas for Medical Sciences, Little Rock, AR*
- TP 542 **Proteomic Analysis of Ancient Dental Calculus Reveals Differences in Host Immune Proteins and Microbiota;** Rosa R. Jersie-Christensen<sup>1</sup>; Anna Fotakis<sup>1,2</sup>; Jan Refsgaard<sup>1</sup>; Christian Kelstrup<sup>1</sup>; Enrico Cappellini<sup>2</sup>; Jesper V. Olsen<sup>1</sup>; <sup>1</sup>*NNF, Center for Protein Research, University of Copenhagen, DK*; <sup>2</sup>*Natural History Museum of Denmark, University of Copenhagen, DK*
- TP 543 **Mass Spectrometric Identification of Amino Acids Modified by 4-hydroxy-2-nonenal (HNE) as a Model for Proteome-Scale Analysis of Oxidative Stress;** Roshanak Aslebagh<sup>1</sup>; Steven J. Fliesler<sup>2,3</sup>; Bruce A. Pfeiffer<sup>2,3</sup>; Costel C. Darie<sup>1</sup>; <sup>1</sup>*Clarkson University, Potsdam, NY*; <sup>2</sup>*SUNY- University at Buffalo, Buffalo, NY*; <sup>3</sup>*VA Western NY Healthcare System, Buffalo, NY*
- TP 544 **Using Advanced Proteome Modeling to Initiate Real-Time Intelligent Time Based Acquisitions;** Scott Geromanos; Steve Ciavarini; *Waters Corporation, Milford, MA*
- TP 545 **Hypoxia-Induced Alternative Splicing Proteomics in Cancer Cell lines;** Liu Chia-Hsiun; Hsu Pang-Hung; , *Keelung, R.O.C.*
- TP 546 **Development of a Generic Proteomics Method Utilizing Self-Optimizing Acquisition Speed on a UHR-QTOF MS;** Stephanie Kaspar<sup>1</sup>; Markus Lubeck<sup>1</sup>; Annette Michalski<sup>1</sup>; Pierre-Olivier Schmit<sup>2</sup>; <sup>1</sup>*Bruker Daltonik GmbH, Bremen, Germany*; <sup>2</sup>*Bruker Daltonique S.A., Wissembourg, France*
- TP 547 **Multiplexed Chemoproteomic Profiling as a Tool to Decipher the Intracellular Interactions between Proteins and Small Molecules Identified in Phenotypic Screens;** Michael Ford<sup>1</sup>; Richard Jones<sup>1</sup>; Ravi Amunugama<sup>1</sup>; Christopher Lietz<sup>2,3</sup>; Danette Daniels<sup>3</sup>; Rachel Ohana<sup>3</sup>; Sergiy Levin<sup>4</sup>; Thomas Kirkland<sup>4</sup>; Marjeta Urh<sup>3</sup>; Keith Wood<sup>3</sup>; <sup>1</sup>*MS Bioworks, Ann Arbor, MI*; <sup>2</sup>*University of Wisconsin, Madison, WI*; <sup>3</sup>*Promega Corporation, Madison, WI*; <sup>4</sup>*Promega Biosciences LLC, San Luis Obispo, CA*
- TP 548 **Proteomic Methods Comparison for Protein Identification and Quantitation of Muscle Proteins;** Jeremy Keirse<sup>1</sup>; Liwen Zhang<sup>1</sup>; Hui Meng<sup>2</sup>; Federica Montanaro<sup>3</sup>; Michael Lawlor<sup>2</sup>; Arpad Somogyi<sup>1</sup>; <sup>1</sup>*Ohio State University, Columbus, Ohio*; <sup>2</sup>*Medical College of Wisconsin, Milwaukee, WI*; <sup>3</sup>*Research Institute-Nationwide Children's Hospital, Columbus, OH*
- TP 549 **Spatiotemporal S-Nitrosoproteome Analysis in Cdk5/p25 Mouse Model of Neurodegeneration by SNOTRAP and Mass Spectrometry;** Uthpala Seneviratne<sup>1</sup>; Ravindra Kodihalli<sup>1</sup>; Vadiraja Bhat<sup>2</sup>; Alexi Nott<sup>1</sup>; John Wishnok<sup>1</sup>; Li-Huei Tsai<sup>1</sup>; Steven Tannenbaum<sup>1</sup>; <sup>1</sup>*Massachusetts Institute of Technology, Cambridge, MA*; <sup>2</sup>*Agilent Technologies, Inc, Wilmington, DE*
- TP 550 **Deciphering Phenotypic Drug Screening Targets Using a Novel Chloroalkane Capture Tag;** Rachel Friedman Ohana<sup>1</sup>; Thomas A. Kirkland<sup>3</sup>; Carolyn C. Woodrooffe<sup>3</sup>; Sergiy Levin<sup>3</sup>; Robin Hurst<sup>1</sup>; Paul Otto<sup>1</sup>; H. Tetsuo Uyeda<sup>3</sup>; Michael Ford<sup>2</sup>; Richard C. Jones<sup>2</sup>; Danette Daniels<sup>1</sup>; Marjeta Urh<sup>1</sup>; Keith Wood<sup>1</sup>; <sup>1</sup>*Promega Corporation, Madison, WI*; <sup>2</sup>*MS Bioworks, LLC, Ann Arbor, MI*; <sup>3</sup>*Promega Biosciences LLC, San Luis Obispo, CA*
- TP 551 **In-Depth Proteome Coverage by Iterative Data Dependent Acquisition on a Benchtop Orbitrap Mass Spectrometer;** Mathias Mueller; Andreas Kuehn; Yue Xuan; Tabiwang N. Arrey; Thomas Rietpietsch; Florian Grosse-Coosmann; Catharina Crone; Torsten Uecker; Markus Kellmann; *Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*
- TP 552 **PERSID: A Proteomic Approach for Identification of S-Sulphydration Sites in Protein Extracts;** Changyuan Lu; Steven S Gross; *Weill Medical College of Cornell, New York, NY*
- TP 553 **Accumulated Ion Monitoring (AIM) Enables Yoctomolar Absolute Sensitivity and Seven Orders of Magnitude Accurate Quantitation in Complex Proteomes;** Paolo Cifani; Avantika Dhabaria; Alex Kentsis; *Memorial Sloan-Kettering Cancer Center, New York, NY*
- TP 554 **Peptides from RNAs Classified as Non-Coding;** Ruchi Chauhan; *Boston Children's Hospital, Neurology, Harvard, Boston, MA*
- TP 555 **Rapid Proteomics Assessment of Toxin Exposed Human Cells to Elucidate Mechanism of Action;** Jamie Allen<sup>1</sup>; Jeffrey Spraggins<sup>1</sup>; Ashley Jordan<sup>1</sup>; William Burns<sup>1</sup>; Jeremy L. Norris<sup>2</sup>; Eric P. Skaar<sup>2</sup>; D. B. Lacy<sup>2</sup>; Richard M. Caprioli<sup>2</sup>; <sup>1</sup>*Vanderbilt University, Nashville, TN*; <sup>2</sup>*Vanderbilt University School of Medicine, Nashville, TN*

**PROTEOMICS:  
NEW APPROACHES – SAMPLE PREPARATION METHODS  
556-586**

- TP 556 **Achieving Optimal Digestion Faster with Flash Digest: Potential Alternative to Multi-Step Detergent Assisted In-Solution Trypsin Digestion in Quantitative and Qualitative Proteomics Experiments;** Vinit Shah; Michael Lassman; Haihong Zhou; Omar Laterza; *Merck Research Laboratories, Rahway, NJ*
- TP 557 **Rapid, Efficient and Reproducible Sample Preparation for Bottom-Up Proteomics by a Surfactant-Aided Precipitation/On-Pellet Digestion Strategy;** Shichen Shen; Jun Li; Xiaomeng Shen; Chengjian Tu; Jun Qu; *SUNY at Buffalo, Buffalo, NY*
- TP 558 **A Routine QC Method to Monitor High-Level LC and MS Performances on Complex Protein Digests;** Stephanie Kaspar<sup>1</sup>; Ole Hoerning<sup>1</sup>; Nicolai Bache<sup>1</sup>; Alexander Harder<sup>1</sup>; Pierre-Olivier Schmit<sup>2</sup>; <sup>1</sup>*Bruker Daltonik GmbH, Bremen, Germany*; <sup>2</sup>*Bruker Daltonique S.A., Wissembourg, France*
- TP 559 **On the Advantages of Admixed Lys-C/Lys-N Digests, for Proteome Depth and DeNovo Peptide Sequencing;** Chris Adams; Anna Okumu; Allis S. Chien; Ryan Leib; *Stanford University Mass Spectrometry, Stanford, CA*
- TP 560 **SPARSE – Streamlined Proteomics And Robust Statistics Experiments: An Optimised Proteomics Pipeline to Increase Analytical Robustness, Accuracy, and Precision;** Ronan O’Cualain; Julian Selley; David Knight; , *M13 9Pt Manchester, UK*
- TP 561 **On-chip Mesoporous Functionalized Magnetic Microspheres for Extended Bottom-Up Proteomics;** Natalia Gasilova; Kristina Srzentic; Liang Qiao; Yury Tsybin; Hubert H. Girault; *EPFL, Lausanne, Switzerland*
- TP 562 **A Simplified Affinity Proteomics Workflow for Rapid, Sensitive, Quantitative Analysis of Proteins in Plasma;** John O’Grady<sup>1</sup>; Kevin Meyer<sup>1</sup>; Michael Stump<sup>2</sup>; Don Gray<sup>2</sup>; <sup>1</sup>*Perfinity Biosciences, Inc, West Lafayette, IN*; <sup>2</sup>*Bioanalytical Systems, Inc, West Lafayette, IN*
- TP 563 **Immuno-Proteomics Using Polyclonal Antibodies and Stable Isotope Labeled Affinity-Purified Recombinant Protein Fragments;** Fredrik Edfors<sup>1,2</sup>; Tove Boström<sup>1</sup>; Masato Habuka<sup>2</sup>; Björn Forsström<sup>1,2</sup>; Mathias Uhlén<sup>1,2</sup>; <sup>1</sup>*Proteomics and Nanobiotechnology, KTH, Stockholm, SE*; <sup>2</sup>*Science for Life Laboratory, KTH, Solna, SE*



- TP 564 **Closer Towards the Native State of Proteomes via Quantum Mechanical Protein Extraction;** Hartmut Schlüter<sup>1</sup>; Marcel Kwiatkowski<sup>1</sup>; Refat Nimer<sup>1</sup>; Marcus Wurlitzer<sup>1</sup>; Sebastian Kruber<sup>2</sup>; Nils-Owe Hansen<sup>2</sup>; R.J. Dwayne Miller<sup>2</sup>; <sup>1</sup>UKE - Mass Spec Proteomics, Hamburg, Germany; <sup>2</sup>MPSD, Hamburg, Germany
- TP 565 **Automated Sample Preparation Solutions for MS-Based Proteomics;** Previn Naicker; Isak Gerber; Justin Jordaan; Stoyan Stoychev; CSIR, Pretoria, South Africa
- TP 566 **FACS-Proteomics: Combining Intracellular Staining, Cell Sorting, and Mass Spectrometry for Proteome Analysis of Targeted Cell Subpopulations;** Tony Ly; Arlene Whigham; Rosemary Clarke; Angus Lamond; Centre for Gene Regulation and Expression, Dundee, UK
- TP 567 **Integrated Strong Cation-Exchange Hybrid Monolith with Capillary Zone Electrophoresis and Mass Spectrometry for Proteomic Analysis;** Zhenbin Zhang; Norman J Dovichi; University of Notre Dame, Notre Dame, IN
- TP 568 **Optimizing Virtual 2D gel/MS through the Analysis of *E. coli* and *M. mazei* Cell Lysate;** Neil R. Quebbemann; Kate Liu; Rachel O. Loo; Joseph A. Loo; University of California, Los Angeles, CA
- TP 569 **Title: Secretome Proteomic Analysis of Stimulated Macrophages Using Metabolic Labeling, Click Chemistry Enrichment, and LC-MS/MS;** Jeffrey Martin; Cheryl Lu; Benbo Gao; Ru Wei; Peter Juhasz; Biogen Idec, Cambridge, MA
- TP 570 **Efficient Desalting and Clean-Up Methods of Protein Digests in Proteomics;** Shota Miyazaki<sup>1</sup>; Naoyuki Sugiyama<sup>2</sup>; Chiaki Aoyama<sup>1</sup>; Kosuke Osaka<sup>1</sup>; Akira Jyukurogi<sup>1</sup>; <sup>1</sup>GL Sciences Inc., Saitama, Japan; <sup>2</sup>Kyoto University, Kyoto, Japan
- TP 571 **Laser Ablation Sample Transfer for Tissue LC-MS/MS Proteomic Investigation;** Fabrizio Donnarumma; Kermit K. Murray; Louisiana State University, Baton Rouge, LA
- TP 572 **On-Bead Digestion - Tackling the challenges of serum proteomics;** Haiyan Zheng<sup>1</sup>; Caifeng Zhao<sup>1</sup>; Meiqian Qian<sup>1</sup>; Swapan Roy<sup>2</sup>; Absari Arpa<sup>2</sup>; Matt Kuruc<sup>2</sup>; <sup>1</sup>Rutgers Center for Proteomics, Piscataway, NJ; <sup>2</sup>Biotech Support Group LLC, Monmouth Junction, NJ
- TP 573 **Optimization of Pulsed Proteolysis Conditions in Plasma Fractions Increases Sequence Coverage and Depth;** Jon Reed<sup>1,2</sup>; Gogce Crynen<sup>1,2</sup>; Prashanthi Vallabhaneni<sup>1</sup>; Rosa Joy<sup>1</sup>; James Evans<sup>1</sup>; Laila Abdullah<sup>1</sup>; Thinh Nguyen<sup>1</sup>; Fiona Crawford<sup>1</sup>; <sup>1</sup>Roskamp Institute, Sarasota, FL; <sup>2</sup>SRQ Bio, Sarasota, FL
- TP 574 **Novel Method for Target Protein Identification Utilizing Immobilized Streptavidin Tips;** Kim Alving; Aharon Cohen; Bing Wang; Genzyme, a Sanofi company, Waltham, MA
- TP 575 **Preparation of Sequence-Controlled Triblock Copolymer-Grafted Silica Microparticles by Sequential-ATRP for Highly Efficient Glycopeptides Enrichment;** Yiting Pan; Weijie Qin; Xiaohong Qian; Beijing Proteome Research Center, Beijing, China
- TP 576 **Identification of Cow Milk-Derived Caseins with Two Dimensional Thin Layer Chromatography Matrix-Assisted Laser Desorption/Ionization Imaging Mass Spectrometry (2D-TLC-MALDI-IMS);** Egidijus Machtejevas<sup>1</sup>; Michael Schulz<sup>1</sup>; Knut Behrend<sup>2</sup>; Sascha Rohn<sup>2</sup>; Katerina Matheis<sup>1</sup>; <sup>1</sup>Merck KGaA, Darmstadt, Germany; <sup>2</sup>University of Hamburg, Hamburg, Germany
- TP 577 **Development of a Sample Enrichment Protocol Using Click Chemistry for Identification of Protein Targets of Reactive Metabolites in Liver Microsomes;** André LeBlanc; Tze Chieh Shiao; René Roy; Lekha Sleno; UQAM, Montréal, Canada
- TP 578 **Cysteine-Selective Dimethylation (cysDML) and Oxidized cysDML (OxycysDML) Methods to Study Redox Signaling in Disease;** Liqing Gu; Renā A. S. Robinson; University Of Pittsburgh, Pittsburgh, PA
- TP 579 **A Hydrophobic Label-Based Depletion Methodology for Enrichment of Protein N-Terminal Peptides from Microgram-Level Samples;** Brian Dill; Joseph Fernandez; Milica Tesic Mark; Henrik Molina; The Rockefeller University, New York, NY
- TP 580 **Chemoselective digestion for middle-down proteomics and structural analysis of monoclonal antibodies;** Kristina Srzentić<sup>1</sup>; Konstantin Zhurov<sup>1</sup>; Gennady Nikitin<sup>1</sup>; Mario Cindrić<sup>2</sup>; Martin Kussmann<sup>1,3</sup>; Yury Tsybin<sup>1</sup>; <sup>1</sup>Ecole Polytechnique Federale, Lausanne, Switzerland; <sup>2</sup>Ruder Boskovic Institute, Zagreb, Croatia; <sup>3</sup>Nestlé Institute of Health Sciences, Lausanne, Switzerland
- TP 581 **Flexible Automated Sample Preparation Workflows: Modified Automated Systems for Specific Immuno-MS and MS Workflows;** David Colquhoun<sup>1</sup>; Mohamed Nazim Boutaghoul<sup>1</sup>; Nishi Rochelle<sup>1</sup>; Brett Noel<sup>2</sup>; Laurie Parker<sup>2</sup>; Kevin W. Meyer<sup>3</sup>; Scott Kuzdzal<sup>1</sup>; Brian Feild<sup>1</sup>; <sup>1</sup>Shimadzu Scientific Instruments, Columbia, MD; <sup>2</sup>University of Minnesota, Minneapolis, MN; <sup>3</sup>Perfinity Biosciences, West Lafayette, IN
- TP 582 **Automated Sample Preparation Workflows for Quantitative Proteomics Applications;** Oliver Popp<sup>1</sup>; Lucas Luethy<sup>2</sup>; Tamara Kanashova<sup>1</sup>; HaAn Nguyen<sup>1</sup>; Julia Kikuchi<sup>1</sup>; Guenter Boehm<sup>2</sup>; Thomas Blenkins<sup>3</sup>; Andreas Bruchmann<sup>3</sup>; Gunnar Dittmar<sup>1</sup>; <sup>1</sup>MDC, Berlin, Germany; <sup>2</sup>CTC Analytics, Zwingen, Switzerland; <sup>3</sup>Axel Semrau GmbH, Sprockhovel, Germany
- TP 583 **High pH Reversed-Phase Peptide Fractionation in a Convenient Spin-Column Format;** Sergei Snovidia<sup>1</sup>; Xiaoyue Jiang<sup>2</sup>; Ramesh Ganapathy<sup>1</sup>; Sijian Hou<sup>1</sup>; Ryan Bomgarden<sup>1</sup>; Paul Haney<sup>1</sup>; Rosa Viner<sup>2</sup>; John C. Rogers<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Rockford, IL; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- TP 584 **MStern Blot - High Throughput PVDF Membrane-Based Proteomic Samples Preparation for 96-Well Plates;** Sebastian Berger<sup>1</sup>; Saima Ahmed<sup>1</sup>; Jan Muntel<sup>1</sup>; Nerea Cuevas Polo<sup>1</sup>; Richard Bachur<sup>2</sup>; Alex Kentsis<sup>3</sup>; Hanno Steen<sup>1</sup>; <sup>1</sup>Harvard Medical School/Children's Hospital Boston, Boston, MA; <sup>2</sup>Boston Children's Hospital, Boston, MA; <sup>3</sup>Cornell University, New York, NY
- TP 585 **Online Membrane-Assisted Buffer Exchanger Coupled with Multijunction Capillary Isoelectric Focusing Device Enables Fractionation of Intact Human Plasma Proteins by pI;** Mohammad Pirmoradian Najafabadi<sup>1,2</sup>; Juan Astorga-Wells<sup>1,2</sup>; Roman A. Zubarev<sup>1</sup>; <sup>1</sup>Karolinska Institutet, Solna, Sweden; <sup>2</sup>Biomotif AB, Stockholm, Sweden
- TP 586 **Automated In-Gel Digestion on a Commercial Autosampler Directly Coupled to Nano LC-MS/MS;** Guenter Boehm<sup>2</sup>; Achermann François<sup>1</sup>; Reto Bolliger<sup>2</sup>; Natasha Buchs<sup>1</sup>; Nicholas Doiron<sup>1</sup>; Sophie Lagache Braga<sup>1</sup>; Manfred Heller<sup>1</sup>; <sup>1</sup>University of Bern, Dpt of Clinical Research, Bern, Switzerland; <sup>2</sup>CTC Analytics AG, Zwingen, Switzerland

**PROTEOMICS:  
QUANTITATIVE – STABLE ISOTOPE LABELING METHODS  
587-605**

- TP 587 **ITMSQ : A Software Tool for Multiple b, y Ion Pairs based Isobaric Tandem Mass Spectrometry Quantification;** Liqi Xie; Lei Zhang; Aiyang Nie; Ying Zhang; Haojie Lu; Fudan university, shanghai, P.R. China
- TP 588 **9-Plex Proteomic Labeling with Neutron-Encoded Amino Acids;** Elyse Freiberger<sup>1</sup>; Anna Merrill<sup>1</sup>; Alex Hebert<sup>1</sup>; William Wood<sup>2</sup>; Marwan ElMasri<sup>2</sup>; Michael S. Westphall<sup>1</sup>; Joel Bradley<sup>2</sup>; Joshua J. Coon<sup>1</sup>; <sup>1</sup>University of Wisconsin, Madison, WI; <sup>2</sup>Cambridge Isotope Laboratories, Inc., Tewksbury, MA
- TP 589 **Performance Evaluation of NeuCode Mouse labeling;** Christopher Rose<sup>1</sup>; Emily Wilkerson<sup>1</sup>; Alan Attie<sup>1</sup>; Joshua Baughman<sup>2</sup>; Joel Bradley<sup>3</sup>; Marwan ElMasri<sup>3</sup>; Alex Hebert<sup>1</sup>;

- TP 590 Mark Keller<sup>1</sup>; Donald S Kirkpatrick<sup>2</sup>; Anna Merrill<sup>1</sup>; Timothy Rhoads<sup>1</sup>; Donald Stapleton<sup>1</sup>; Michael S. Westphall<sup>1</sup>; Clay Williams<sup>1</sup>; William Wood<sup>3</sup>; Joshua J. Coon<sup>1</sup>; <sup>1</sup>University of Wisconsin, Madison, WI; <sup>2</sup>Genentech, Inc., South San Francisco, CA; <sup>3</sup>Cambridge Isotope Labs., Andover, MA  
**Developmental Phosphoproteomics Identifies Casein Kinase 2 as a Therapeutic Target in Medulloblastoma;** Teresa Purzner<sup>1</sup>; John Sanders<sup>1</sup>; Tom Hartl<sup>1</sup>; James Purzner<sup>1</sup>; Yoon-Jae Cho<sup>1</sup>; Josh Elias<sup>1</sup>; Matthew Scott<sup>2</sup>; <sup>1</sup>Stanford University, Stanford, CA; <sup>2</sup>Carnegie Institution for Science, Washington, DC
- TP 591 **Mapping Proteolytic Peptide Production Rates in Plasma Using Stable Isotope Labeled Proteins from the SILAC-Labeled HepG2 Secretome;** John B. Mangrum; Erika J. Martin; Donald F. Brophy; Adam M. Hawkrige; <sup>Virginia Commonwealth University, Richmond, VA</sup>
- TP 592 **Quantitation of Methylation Levels in Specifically-Modified Histone H3 Standards by Stable-isotope Labeling and Mass Spectrometry;** Steven Toth; Wendell P. Griffith; , Toledo, OH
- TP 593 **Identification of p53-Induced Changes to the Non-Small Cell Lung Cancer Proteome;** Emmanuel Cudjoe; Khushboo Sharma; John Mangrum; David Gewirtz; Adam Hawkrige; <sup>Virginia Commonwealth University, Richmond, Virginia</sup>
- TP 594 **PCSK9 and Its Variants: A Global Proteomic Study to Identify Interactors and Effects on Protein Trafficking;** Ge Chu; Zhibin Ning; Janice Mayne; Daniel Figeys; <sup>University of Ottawa, Ottawa, ON</sup>
- TP 595 **In-Depth Comparative Mapping of the Global Proteome between Primary and Metastatic Skin Melanoma Cells Derived from the Same Individual;** Lei Guo; Weili Miao; Yongsheng Xiao; Yinsheng Wang; <sup>University of California, Riverside, Riverside, CA</sup>
- TP 596 **Quantitative Proteomics Deciphers Druggable ALK Signaling in Neuroblastoma;** Kristina B. Emdal; Anna-Kathrine Pedersen; Dorte B. Bekker-Jensen; Chiara Francavilla; Jesper V. Olsen; <sup>The NNF Center for Protein Research, Copenhagen, Denmark</sup>
- TP 597 **Quantification of the Membrane Differential Proteomes by Stable Isotope Labeling and Spectral Counting Strategies;** Ying Wai Lam<sup>1,2</sup>; Bin Deng<sup>1,2</sup>; Julia Fields<sup>1,2</sup>; Kenneth Smith<sup>1</sup>; Richard Voogt<sup>1</sup>; Keith Mintz<sup>1</sup>; <sup>1</sup>University of Vermont, Burlington, VT; <sup>2</sup>UVM/VGN Proteomics Facility, Burlington, VT
- TP 598 **Quantitative Proteomic Profiling of the Newly Synthesized Proteins Associated with T Cell Growth;** Qing Kong; Zengli Guo; Xin Wei; Cui Liu; Xian Chen; Yisong Wan; <sup>University of North Carolina at Chapel Hill, Chapel Hill, NC</sup>
- TP 599 **Systematic Investigation of Cellular Response and Pleiotropic Effects in Atorvastatin-treated Liver Cells by MS-based Proteomics;** Haopeng Xiao; Weixuan Chen; George Tang; Johanna Smeekens; Ronghu Wu; <sup>Georgia Institute of Technology, Atlanta, GA</sup>
- TP 600 **Characterization of Progression-Related Signaling Networks in a Colon Cancer Metastasis Model Using Phosphoproteomics;** Alissa Schunter; Xiaoshan Yue; Amanda B. Hummon; <sup>University of Notre Dame, Notre Dame, IN</sup>
- TP 601 **Mass Defect-Based Pseudo-Isobaric a1 Ion Pairs Enabled Accurate Proteome Quantification with Wide Dynamic Range and Deep Coverage;** Yuan Zhou; Jianhui Liu; Lihua Zhang; Yukui Zhang; <sup>Dalian Institute of Chemical Physics, Dalian, China</sup>
- TP 602 **In vitro Metabolic Labeling of Human Gut Microbiota for Quantitative Metaproteomics;** Xu Zhang; Zhibin Ning; Janice Mayne; Alain Stintzi; Daniel Figeys; <sup>Ottawa Institute of Systems Biology, Ottawa, Canada</sup>
- TP 603 **Application of Stable Isotope-Labeled Protein Fragments to Investigate the Correlation of Protein and mRNA Levels in Human Cell Lines;** Tove Boström<sup>1</sup>; Frida Danielsson<sup>2</sup>; Emma Lundberg<sup>2</sup>; Henrik J Johansson<sup>3</sup>; Hanna Tegel<sup>4</sup>; Janne Lehtiö<sup>3</sup>; Mathias Uhlén<sup>2</sup>; Sophia Hober<sup>1</sup>; Jenny Ottosson Takanen<sup>4</sup>; <sup>1</sup>Department of Protein Technology, KTH, Stockholm, Sweden; <sup>2</sup>Science for Life Laboratory, KTH, Stockholm, Sweden; <sup>3</sup>Science for Life Laboratory, KI, Stockholm, Sweden; <sup>4</sup>Department of Proteomics, KTH, Stockholm, Sweden
- TP 604 **Targeted Absolute Quantification of Protein by GeLC-MS/MS: Western Blot Takes the Back Seat;** Mukesh Kumar<sup>1</sup>; Shai Joseph<sup>1</sup>; Martina Augsburg<sup>2</sup>; David Drechsel<sup>1</sup>; Nadine Vastenhouw<sup>1</sup>; Frank Buchholz<sup>2</sup>; Marc Gentzel<sup>1</sup>; Andrej Shevchenko<sup>1</sup>; <sup>1</sup>MPI-CBG, Dresden, Dresden, Germany; <sup>2</sup>Medical Systems Biology Medical Faculty, TU Dresden, Dresden, Germany
- TP 605 **Characterization of Clinically-Relevant Stable Isotope Labeled Recombinant Proteins For Use As Internal Standards in Quantitative MS Workflows;** Kevin Ray; Pegah Jalili; David Rhee; Yongsheng Xiao; James J. Walters; <sup>Sigma-Aldrich, St. Louis, MO</sup>
- BIOMARKER: QUANTITATIVE ANALYSIS (NON-PROTEIN, LIPIDS/METABOLITES/COMPOUNDS)  
606-629**
- TP 606 **Renal Cell Carcinoma Biomarker Screening by High-Performance Liquid Chromatography - Tandem Mass Spectrometry;** Sisi Chen<sup>1</sup>; Casey Burton<sup>1</sup>; Anthony Kaczmarek<sup>2</sup>; Honglan Shi<sup>1</sup>; Yinfa Ma<sup>1</sup>; <sup>1</sup>Missouri University of Science and Technology, Rolla, MO; <sup>2</sup>Central Missouri Urology Clinic, Rolla, MO
- TP 607 **A Fit-for-Purpose LC-MS/MS Method for the Quantitative Measurement of Creatinine in Human Plasma;** Yue Zhao; Guowen Liu; Aida Angeles; Lisa Christopher; Xuewen Ma; Jim Shen; Mark Arnold; <sup>Bristol-Myers Squibb Co., Princeton, NJ</sup>
- TP 608 **The analysis of Sweat Biomarkers in Mechanically-Loaded Tissues Using SFC-MS;** Julie Herriman<sup>1</sup>; G. John Langley<sup>1</sup>; Rachel Greenhill<sup>1</sup>; Peter Worsley<sup>2</sup>; Dan Bader<sup>2</sup>; Tim Jenkins<sup>3</sup>; <sup>1</sup>Chemistry, University of Southampton, Southampton, UK; <sup>2</sup>Health Sciences, University of Southampton, Southampton, UK; <sup>3</sup>Waters Corporation, Wilmslow, UK
- TP 609 **Method Development for the Determination of 24S-Hydroxycholesterol in Human Plasma by LC/APCI-MS/MS;** Hiroshi Sugimoto; Masaaki Kakehi; Yoshinori Satomi; Hidenori Kamiguchi; Fumihito Jinno; <sup>Takeda Pharmaceutical Company Limited, Fujisawa, Japan</sup>
- TP 610 **Rapid and Selective Determination of 3-Nitrotyrosine in Human Blood Plasma;** Oleg Timofeev<sup>1</sup>; Jin Ji<sup>2</sup>; <sup>1</sup>Zintro Consulting, Monmouth Jct, NJ; <sup>2</sup>Brunswick Laboratories, Inc., Southborough, MA
- TP 611 **Quantification of Heparan Sulphate in Mucopolysaccharidoses Patient Urines using Novel Butanolysis Depolymerisation/Desulphation Sample Work-Up;** Paul Trim; John Hopwood; Marten Snel; <sup>South Australian Health & Medical Research Inst., Adelaide, AUSTRALIA</sup>
- TP 612 **A Sensitive LC-MS/MS Method for Quantitation of 7 $\alpha$ -hydroxy-4-cholesten-3-one in Human Plasma;** Dawei Zhou; Xingye Yang; Manik Desai; Jinn Wu; Xinping Fang; <sup>XenoBiotic Laboratories, Inc., WuXi AppTec, Inc., Plainsboro, NJ</sup>
- TP 613 **Noninvasive Measurement of Aristolochic Acid-DNA Adducts in Urine Samples from Rats by Liquid Chromatography Coupled Electrospray Ionization Tandem Mass Spectrometry;** Elvis Leung; <sup>HKUST, Hong Kong, China</sup>



- TP 614 **Determination of Endogenous Cortisol in Human Plasma Using LC-MS/MS Techniques with A Combined Calibration Curve and Standard Addition Methods;** Yansheng Liu<sup>1</sup>; Yu-Hui Fu<sup>1</sup>; David Winburn<sup>1</sup>; Rodney Boughner<sup>1</sup>; Stephen Wanaski<sup>2</sup>; Daniel Selness<sup>3</sup>; Gene Ray<sup>1</sup>; <sup>1</sup>KCAS LLC, Shawnee, KS; <sup>2</sup>Marathon Pharmaceuticals, LLC, Northbrook, IL; <sup>3</sup>Spaulding Clinical Research, West Bend, WI
- TP 615 **Aspects of Electrospray Ionization of 25 Hydroxy Vitamin D. Lessons Learned;** Eduard Rogatsky; Daniel Stein; *Albert Einstein College of Medicine, Bronx, NY*
- TP 616 **LC-MS/MS Bioanalytical Support of Mouse Serial Microsampling Studies via Extraction of Sub-Microliter Volumes: Examples Including the Biomarker S-Adenosylmethionine;** Bao Hoang; Eric Britton; Casey Bonner; Danielle Pessolano; Sean Maki; Rick Luzietti; Angela Qi Shen; Steven Wiltshire; *Agilux Laboratories, Worcester, MA*
- TP 617 **Using HILIC to Improve LC-MS Sensitivity for the Detection of DNA Adducts Derived from Tobacco Specific N-Nitrosamines;** Lucie Loukotkova; Lei Guo; Frederick Beland; Goncalo Gamboa Da Costa; *NCTR, US FDA, Jefferson, AR*
- TP 618 **The Ratio of 8-iso-prostaglandin F2 $\alpha$  to Prostaglandin F2 $\alpha$  Distinguishes Enzymatic from Nonenzymatic Isoprostane Formation;** Fred Bjorn Lih; Thomas J. van 't Erve; Thomas E. Eling; Maria B. Kadliiska; Ronald P. Mason; Leesa J. Deterding; *NIEHS / NIH, RTP, NC*
- TP 619 **Measurement of Flame Retardant Metabolites in Human Urine by Solid Phase Extraction- Ultra High Performance Liquid Chromatography-Tandem Mass Spectrometry;** Nayana K. Jayatilaka; Paula Restrepo; Antonia M. Calafat; Liza Valentín-Blasini; *Centers for Disease Control and Prevention, Atlanta, GA*
- TP 620 **Development of a High-Sensitivity Micro LC/MS Method for Estradiol Quantification in Human Plasma;** Angela Doneanu<sup>1</sup>; James Murphy<sup>2</sup>; <sup>1</sup>Waters, Milford, MA; <sup>2</sup>Waters Corporation, Milford, MA
- TP 621 **A Robust and Efficient Approach to Quantitation of Organic Acids in Biological Matrices;** Vikki Tsefrikas; Kyle Goodsell; Dylan Bennett; Allysen Meymaris; *Agilux Laboratories, Worcester, MA*
- TP 622 **Quantification of Monohydroxy-Polycyclic Aromatic Hydrocarbons (OH-PAHs) in Urine by Online SPE-HPLC-MS/MS;** Yuesong Wang; Lei Meng; Erin Pittman; Alisha Etheredge; Kendra Hubbard; Debra Trinidad; Kayoko Kato; Xiaoyun Ye; Antonia Calafat; *CDC, Atlanta, GA*
- TP 623 **A SWATH-MS Approach to the Secretome under Oxidative Stress Conditions: Proteins and Metabolites Unravelled;** Sandra Anjo<sup>1,2</sup>; Vera Mendes<sup>1</sup>; Mário Grãos<sup>1</sup>; Bruno Manadas<sup>1</sup>; <sup>1</sup>Center for Neuroscience and Cell Biology, Cantanhede, Portugal; <sup>2</sup>Faculty of Sciences and Technology, Coimbra, Portugal
- TP 624 **A Multi-Marker Panel for Measuring Oxidative Stress in Tissue Samples Using LC/MS/MS;** Hideji Fujiwara; Christopher Holley; David Scherrer; Rohini Sidhu; Daniel Ory; Jean Schaffer; *Washington University School of Medicine, St. Louis, MO*
- TP 625 **High-Throughput Intracellular Pteridinic Profiling by Liquid Chromatography – Quadrupole Time-of-Flight Mass Spectrometry;** Casey Burton<sup>1</sup>; Rui Weng<sup>2</sup>; Li Yang<sup>2</sup>; Yu Bai<sup>2</sup>; Huwei Liu<sup>2</sup>; Yinfa Ma<sup>1</sup>; <sup>1</sup>Missouri University of Science and Technology, Rolla, Missouri; <sup>2</sup>Peking University, Beijing, China
- TP 626 **Quantification of Quorum Sensing Molecules and their Interaction with Polymixin-B Hemoperfusion in Human Plasma by LC-HRMS;** Claudio Medana; Federica Dal Bello; Valentina Santoro; Chiara Martano; Davide Medica; Alessandro Quercia; Vincenzo Cantaluppi; *University of Turin, Torino, Italy*
- TP 627 **Measurement of Catecholamines in Rat and Mini-pig Plasma and Urine by Liquid Chromatography-Tandem Mass Spectrometry Coupled with Solid Phase Extraction;** Huaibing He; Ester Carballo-Jane; Xinchun Tong; Lucinda Cohen; *Merck & Co., Inc., Rahway, NJ*
- TP 628 **Towards a Multi-Analyte, High Dynamic Range, High Throughput LC/MS/MS Smoker Screening Method;** Vincent Pagnotti; June Feng; Lanqing Wang; Benjamin Blount; *U.S. Centers for Disease Control and Prevention, Atlanta, GA*
- TP 629 **Analysis of Radiation-Induced Injury by Targeted High-Throughput Metabolomics;** Jace W. Jones<sup>1</sup>; Claire L Carter<sup>1</sup>; Gregory Tudor<sup>2</sup>; Alexander Bennett<sup>1</sup>; Ann Farese<sup>1</sup>; Isabel L Jackson<sup>1</sup>; Zeljko Vujaskovic<sup>1</sup>; Catherine Booth<sup>2</sup>; Thomas J MacVittie<sup>1</sup>; Maureen A Kane<sup>1</sup>; <sup>1</sup>University of Maryland, Baltimore, MD; <sup>2</sup>Epistem, Ltd., Manchester, UK

#### DISEASE BIOMARKERS 630-654

- TP 630 **Defining Molecular Mechanisms for the Anti-Colon Cancer Activity of Anthocyanin-containing Purple-fleshed Potato: A Shotgun Proteomic Approach;** Jairam Vanamala<sup>1,2</sup>; Venkata Charepalli<sup>1</sup>; Sridhar Radhakrishnan<sup>1</sup>; Vadiraja Bhat<sup>3</sup>; Lavanya Reddivari<sup>1</sup>; <sup>1</sup>Pennsylvania State University, University Park, PA; <sup>2</sup>The Penn State Hershey Cancer Institute, Hershey, PA; <sup>3</sup>Agilent Technologies, Wilmington, DE
- TP 631 **From Metabolomic Phenotyping Data to Clinical Signatures;** Guido Krebiehl; Guido Dallmann; Therese Koal; Wulf Fischer-Knuppertz; *Biocrates Life Sciences AG, Innsbruck, Austria*
- TP 632 **Proteomics Profiling and Potential Biomarker Detection in Sjogren's Syndrome after Ultrasound-Assisted Gene Transfer of IL-17R:Fc Chimera;** Changgong Wu<sup>1</sup>; Zhimin Wang<sup>1</sup>; Lee Zourelis<sup>1</sup>; Hiteshi Thakker<sup>2</sup>; Michael Passineau<sup>1</sup>; <sup>1</sup>Allegheny General Hospital, Pittsburgh, PA; <sup>2</sup>Greentree Medical Associates, Pittsburgh, PA
- TP 633 **Mass Spectrometry Based Proteomics for Absolute Quantification of Proteins from Tumor Cells;** Hong Wang; Sam Hanash; *MD Anderson Cancer Center, Houston, TX*
- TP 634 **A Quantitative Proteomics Study of Cerebrospinal Fluid from Individual Niemann-Pick Disease, Type C1 Patients;** Stephanie M. Cologna<sup>1</sup>; Brian C. Searle<sup>2</sup>; Paul S. Blank<sup>1</sup>; Christopher A. Wassif<sup>1</sup>; Nicole M. Yanjanin<sup>1</sup>; Peter S. Backlund<sup>1</sup>; Alfred L. Yerger<sup>1</sup>; <sup>1</sup>National Institutes of Health, Bethesda, MD; <sup>2</sup>Proteome Software Inc., Portland, OR
- TP 635 **Identification of Stroke Metalloprotein Biomarkers and Metal Profile in Human Blood Plasma for Specialized Treatment;** Keaton Nahan<sup>1</sup>; Julio Landero Figueroa<sup>1</sup>; Opeolu Adeoye<sup>2</sup>; Joseph Caruso<sup>1</sup>; <sup>1</sup>Dept of Chemistry, University of Cincinnati, Cincinnati, Ohio; <sup>2</sup>Medical Center, University of Cincinnati, Cincinnati, OH
- TP 636 **Identification of Moesin as a New Endothelial Marker in Human Sepsis Using SILAC-Based Secretomics;** Oh Kwang Kwon<sup>1</sup>; Sae-kwang Ku<sup>2</sup>; Wonhwa Lee<sup>1</sup>; Sunju Kim<sup>1</sup>; Joung A Kim<sup>1</sup>; Jin Young Kim<sup>3</sup>; Shin-Woo Kim<sup>1</sup>; Sangkyu Lee<sup>1</sup>; <sup>1</sup>Kyungpook National University, Daegu, Republic Of Korea; <sup>2</sup>Daegu Haany University, Gyeongsan-si, Republic Of Korea; <sup>3</sup>Korea Basic Science Institute, Ochang, Republic Of Korea
- TP 637 **Identification of Early Proteomic Biomarkers of Nonclinical Cardiotoxicity;** Li-Rong Yu; Zhijun Cao; Yuan Gao; Richard Beger; James Fuscoe; Varsha Desai; *National Center for Toxicological Research, FDA, Jefferson, AR*
- TP 638 **Revealing Pathways In COPD-Associated Lung Cancer Via Large-Scale Quantitative Multi-omic Analysis;** Brian J Sandri<sup>1</sup>; Andy H Limper<sup>2</sup>; Pratik Jagtap<sup>3</sup>; Svetlana V Avdulov<sup>1</sup>; Mark S Peterson<sup>1</sup>; Carl Murie<sup>4</sup>; Yang Ping<sup>2</sup>; Ola Larsson<sup>4</sup>; Peter B Bitterman<sup>1</sup>; Leeann Higgins<sup>3</sup>; Todd

- W Markowski<sup>3</sup>; Tim J Griffin<sup>3</sup>; Chris H Wendt<sup>1,5</sup>; <sup>1</sup>University of Minnesota, Minneapolis, MN; <sup>2</sup>Mayo Clinic, Rochester, MN; <sup>3</sup>Center for Mass Spectrometry and Proteomics, UMN, St. Paul, MN; <sup>4</sup>Karolinska Institute, Solna, Sweden; <sup>5</sup>VA Medical Center, Minneapolis, MN
- TP 639 **NASH Mechanism Understanding Using MS Imaging: Discover New Disease State Biomarkers;** Pierre-Maxence Vaysse<sup>1</sup>; Anita M. van den Hoek<sup>2</sup>; Gregory Hamm<sup>1</sup>; Robert Kleemann<sup>2</sup>; Jonathan Stauber<sup>1</sup>; Hans M.G. Princen<sup>2</sup>; <sup>1</sup>ImaBiotech, MS Imaging Dept., Loos, France; <sup>2</sup>TNO, Metabolic Health Research, Leiden, The Netherlands
- TP 640 **Development of Multi-Marker Diagnostic Platforms for Early Diagnosis of Hepatocellular Carcinoma;** Areum Sohn; , Seoul, South Korea
- TP 641 **Proteomic Identification of Head and Neck Cancer Patients with Persistent Human Papillomavirus Infections Associated with Improved Survival;** Nicolas Schlecht<sup>1</sup>; Nicole Kawachi<sup>1</sup>; Yanhua Wang<sup>1,3</sup>; Thomas Harris<sup>1</sup>; Thomas Belbin<sup>1</sup>; Peicheng Du<sup>2</sup>; Richard Smith<sup>3</sup>; Ruth Angeletti<sup>1</sup>; Michael Prystowsky<sup>1</sup>; Jihyeon Lim<sup>1</sup>; <sup>1</sup>Albert Einstein College of Medicine, Bronx, NY; <sup>2</sup>Rutgers University, Newark, NJ; <sup>3</sup>Montefiore Medical Center, Bronx, NY
- TP 642 **A Simple and Sensitive Method for the Analysis of Sphingolipid Glycosylation Enables the Differentiation of Ovarian Cancer Sub-Types;** Arun Everest-Dass; Merrina Anugraham; Nicolle Packer; *Macquarie University, Sydney, Australia*
- TP 643 **Determination of Polyp & Cancer-free Resection Margins in Colonoscopy, Complex Pelvic and Colonic Surgery using Rapid Evaporative Ionization Mass Spectrometry;** James L Alexander<sup>1</sup>; Julia Balog<sup>1,2</sup>; Alasdair J Scott<sup>1</sup>; Abigail VM Speller<sup>1</sup>; Laura J Muirhead<sup>1</sup>; James Kinross<sup>1</sup>; Julian P Teare<sup>1</sup>; Zoltan Takats<sup>1</sup>; <sup>1</sup>Imperial College London, London, UK; <sup>2</sup>Waters Corporation, Wilmslow, UK
- TP 644 **Development of a MS Assay to Identify Breast Cancer Candidate Biomarkers from Formalin-Fixed Paraffin Embedded (FFPE) Tissue;** Ten-Yang Yen; Moe Thein; Roger Yen; Leslie Timpe; Bruce Macher; *San Francisco State University, San Francisco, CA*
- TP 645 **Protein Profile of *Schistosoma mekongi* using GeLC-MS/MS Based Proteomics;** Onrapak Reamtong<sup>1</sup>; Polkit Sangvanich<sup>2</sup>; Supaporn Supaporn Nuamtanong<sup>1</sup>; Phiraphol Chusongsang<sup>1</sup>; Poom Adisakwattana<sup>1</sup>; <sup>1</sup>Mahidol University, Bangkok, Thailand; <sup>2</sup>Chulalongkorn University, Bangkok, Thailand
- TP 646 **Diagnosis of Lung Tumor Types Based on Metabolomic Profiles in Lymph Node Aspirates;** Daniel Sappington; , Little Rock, AR
- TP 647 **Proteomic and Transcriptomic Profiling of an Inducible Model of Acute Myeloid Leukemia Reveals Novel Insights into Leukemogenesis;** Jarrod Sandow; Gabriella Brumatti; Giuseppe Infusini; Paul Ekert; Andrew Webb; *The Walter & Eliza Hall Institute, Parkville, Australia*
- TP 648 **The Oxidized Proteome of Peripheral Blood Mononuclear Cells: A Valuable Repository for Clinical Proteomics;** Daniel Lopez Ferrer; Xiaolei Xie; Xiaoyue Jiang; Andreas Huhmer; *Thermo Fisher Scientific, San Jose, CA*
- TP 649 **Method for the Analysis of Neurosteroids in Human Serum to a LLOQ of 5 pg/mL;** Vince Windisch<sup>1</sup>; John Slemmon<sup>2</sup>; John Masucci<sup>2</sup>; Allan Xu<sup>1</sup>; <sup>1</sup>Keystone Bioanalytical, Inc., North Wales, PA; <sup>2</sup>Janssen Research and Development, Spring House, PA
- TP 650 **The Quantitation of Glucosylsphingosine in Mouse Models of Gaucher Disease by Liquid Chromatography-Tandem Mass Spectrometry;** Rick Hamler<sup>1</sup>; Nastry Brignol<sup>1</sup>; Sean Morrison<sup>1</sup>; Angela Sanders<sup>2</sup>; Leo Dungan<sup>1</sup>; Hui Hwa Chang<sup>1</sup>; Kenneth J. Valenzano<sup>1</sup>; Robert E. Boyd<sup>1</sup>; Chau Dang<sup>1</sup>; Lorne A. Clarke<sup>2</sup>; Sean W. Clark<sup>1</sup>; Elfrida R. Benjamin<sup>1</sup>; <sup>1</sup>Amicus Therapeutics, Cranbury, NJ; <sup>2</sup>Dept of Medical Genetics, Univ of British Columbia, British Columbia, Canada
- TP 651 **Accurate Quantitation of Plasma Globotriaosylsphingosine (lyso-Gb3) in Healthy Individuals and Fabry Patients by Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS);** Rick Hamler<sup>1</sup>; Nastry Brignol<sup>1</sup>; Robert Boyd<sup>1</sup>; Daniel G. Bichet<sup>2</sup>; Dominique P. Germain<sup>3</sup>; Roberto Giugliani<sup>4</sup>; Derrilyn A. Hughes<sup>5</sup>; Raphael Schiffmann<sup>6</sup>; William R. Wilcox<sup>7</sup>; Hadis N. Williams<sup>1</sup>; Julie Yu<sup>1</sup>; Jay Barth<sup>1</sup>; Jeff Castelli<sup>1</sup>; Kenneth J. Valenzano<sup>1</sup>; Jeff Castelli<sup>1</sup>; Elfrida R. Benjamin<sup>1</sup>; <sup>1</sup>AMICUS Therapeutics, Paoli, PA; <sup>2</sup>Hôpital du Sacré-Coeur, Montreal, Quebec, Canada; <sup>3</sup>Hôpital Raymond Poincaré, University of Versailles, Garches, France; <sup>4</sup>Medical Genetics Service, HCPA/UFRGS, Porto Alegre, Brazil; <sup>5</sup>Royal Free Campus, University College London, London, UK; <sup>6</sup>Baylor Research Institute, Dallas, Dallas, TX; <sup>7</sup>Department of Human Genetics, Emory University, Atlanta, GA
- TP 652 **Absolute Quantitation of Apolipoprotein E3 and E4 Isoforms from Human Cerebrospinal Fluid and Brain;** Alaina Baker-Nigh<sup>1</sup>; Kwasi Mawuenyega<sup>1</sup>; Vitaliy Ovod<sup>1</sup>; Hamideh Zakeri<sup>1</sup>; Tom Kasten<sup>1</sup>; Randall Bateman<sup>1,2</sup>; <sup>1</sup>Washington University School of Medicine, Saint Louis, MO; <sup>2</sup>Knight Alzheimer's Disease Research Center, St. Louis, MO
- TP 653 **SWATH Analysis of Patient-Derived iPSC to Motor Neurons for the Discovery of Protein Network Perturbations that Underlie Motor Neuron Diseases;** Andrea Matlock; Loren Ornelas; Ronald Holewinski; Berhan Mandefro; Lindsay Lenaeus; Anais Sahabian; Clive Svendsen; Dhruv Sareen; Jennifer E. Van Eyk; *Cedars-Sinai, Los Angeles, CA*
- TP 654 **Detection of Breast Cancer Recurrence Using LC-MS/MS Targeted Metabolic Profiling;** Jiangjiang Zhu<sup>1</sup>; Lingli Deng<sup>1,3</sup>; Danijel Djukovic<sup>1</sup>; Haiwei Gu<sup>1</sup>; Daniel Rafferty<sup>1,2</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Fred Hutchinson Cancer Research Center, Seattle, WA; <sup>3</sup>Xiamen University, Xiamen, China

#### IMAGING MS: PHARMACEUTICAL APPLICATIONS 655-667

- TP 655 **Utility of High Resolution MALDI Imaging in Drug Discovery: Histological Distribution of Gentamicin in Proximal Renal Tubules of Rats;** Hidefumi Kaji<sup>1</sup>; Hiroyuki Hashimoto<sup>1</sup>; Masayoshi Saito<sup>1</sup>; Takushi Yamamoto<sup>2</sup>; Noriyuki Ojima<sup>2</sup>; <sup>1</sup>Mitsubishi Tanabe Pharma Corporation, Saitama, Japan; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan
- TP 656 **MALDI-Imaging Mass Spectrometry for Pharmacokinetics of Transcutaneous Medicine;** Eishi Imoto; *Osaka University, Suita City, Japan*
- TP 657 **Blocking NMDA Mediated DYN Neurotoxicity influences Brain Lipids Profile in Traumatic Brain Injury;** Amina S. Woods<sup>1</sup>; Shelley N Jackson<sup>1</sup>; Aurelie Roux<sup>1</sup>; Ludovic Muller<sup>1</sup>; J Albert Schultz<sup>2</sup>; Brian M Cox<sup>3,4</sup>; Carey Balaban<sup>5</sup>; <sup>1</sup>NIDA-IRP, NIH, Baltimore, MD; <sup>2</sup>Ionwerks, Inc., Houston, TX; <sup>3</sup>Uniformed Services University, Bethesda, MD; <sup>4</sup>Center for Neuroscience and Regenerative Medicine, Rockville, MD; <sup>5</sup>University of Pittsburgh, Pittsburgh, PA
- TP 658 **Visualizing Brimonidine Distribution in Pig Optic Nerve Tissue by Imaging Mass Spectrometry;** Michelle Reyzer; Chad Chumbley; Michael DeLisi; Louise Mawn; Eva Harth; Robert Galloway; Richard Caprioli; *Vanderbilt University, Nashville, TN*
- TP 659 **Small Molecule Analysis in Single Hair Strands for Evaluation of Drug Adherence with IR-MALDESI MSI;** Elias Rosen<sup>1</sup>; Corbin Thompson<sup>2</sup>; Mark Bokhart<sup>1</sup>; Heather





- Prince<sup>2</sup>; Craig Sykes<sup>2</sup>; Angela DM Kashuba<sup>2</sup>; David C. Muddiman<sup>1</sup>; <sup>1</sup>North Carolina State University, Raleigh, NC; <sup>2</sup>University of North Carolina, Chapel Hill, NC
- TP 660 **Mass Spectrometry Imaging of the Fly Brain**; Andrew Ewing<sup>1,2</sup>; Nhu Phan<sup>2</sup>; John Fletcher<sup>1</sup>; <sup>1</sup>Chalmers University, Gothenburg, Sweden; <sup>2</sup>University of Gothenburg, Gothenburg, Sweden
- TP 661 **Under the skin: Biomarkers of Cutaneous Defenses to Vaccines using Mass Spectrometry Imaging**; Juliette Masure<sup>1</sup>; Hélène Perrin<sup>2</sup>; Gregory Hamm<sup>1</sup>; Maxence Wisztorski<sup>4</sup>; Melody Dufossé<sup>2</sup>; Charlotte Primard<sup>3</sup>; Jean-Pierre Both<sup>5</sup>; Michel Salzet<sup>4</sup>; Isabelle Fournier<sup>4</sup>; Anthony Larue<sup>5</sup>; Jonathan Stauber<sup>1</sup>; Béhazine Combadière<sup>2</sup>; <sup>1</sup>ImaBiotech, MS Imaging Dept., Loos, France; <sup>2</sup>INSERM U1135-Cimi-Paris, Paris, France; <sup>3</sup>Adjuvatis, Lyon, Lyon; <sup>4</sup>PRISM Lab. INSERM U1192, Univ. Lille1, Villeneuve d'Ascq, France; <sup>5</sup>CEA-List, Gif-sur-Yvette, France
- TP 662 **Distribution of Newly Coordinated <sup>57</sup>Fe-heme by MALDI FT-ICR MS Imaging Proved the Efficacy of Epoetin Beta Pegol (C.E.R.A.)**; Makoto Kihara; Mariko Noguchi-Sasaki; Yukari Matsuo-Tezuka; Keigo Yorozu; Mitsue Kurasawa; Hideyuki Yasuno; Yasushi Shimonaka; *Chugai Pharmaceutical Co., Ltd, Kamakura, Japan*
- TP 663 **Blood-Brain Barrier Drug Targeting by Mass Spectrometry Imaging in Early Adme Profiling**; Theodosia Vallianatou<sup>1</sup>; Henrik Loden<sup>1</sup>; Anna Nilsson<sup>1</sup>; Mohammadreza Shariatgorji<sup>1</sup>; Marcela Pereira<sup>2</sup>; Per Svenningsson<sup>2</sup>; Maria Karlgren<sup>1</sup>; Per E. Andren<sup>1</sup>; <sup>1</sup>Uppsala University, Uppsala, Sweden; <sup>2</sup>Karolinska Institute, Stockholm, Sweden
- TP 664 **MALDI-IMS-MSI for the Analysis of 3D Tissue-Engineered Psoriatic Skin Models**; Amanda Harvey<sup>1</sup>; Laura Cole<sup>1</sup>; John Warwick<sup>2</sup>; Richard Bojar<sup>2</sup>; David Smith<sup>1</sup>; Neil Cross<sup>1</sup>; Malcolm Clench<sup>1</sup>; <sup>1</sup>Sheffield Hallam University, BMRC, Sheffield, UK; <sup>2</sup>Innovenn, York, UK
- TP 665 **Mass Spectrometry Imaging of Drug Related Crystal-Like Structures in Frozen and Paraffin Embedded Rabbit Kidney Tissue Sections**; Anne L. Bruinen<sup>1,2</sup>; Ronald de Vries<sup>3</sup>; Marjolein van Heerden<sup>3</sup>; Rob J. Vreeken<sup>3</sup>; Filip Cuyckens<sup>3</sup>; Ron M.A. Heeren<sup>1,2</sup>; <sup>1</sup>FOM Institute AMOLF, Amsterdam, Netherlands; <sup>2</sup>M4I, Maastricht University, Maastricht, NL; <sup>3</sup>Janssen Pharmaceutica, Beerse, Be
- TP 666 **Validating Quantitative Imaging Mass Spectrometry of Pharmaceuticals in Tissue Sections**; Chad Chumbley<sup>1</sup>; Michelle Reyzer<sup>1</sup>; Gwendolyn Marriner<sup>2</sup>; Laura Via<sup>2</sup>; Clifton Barry III<sup>2</sup>; Richard Caprioli<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>NIH/NIAD, Bethesda, MD
- TP 667 **A Nanostructured Matrices Assessment to Study Drugs Distribution in Solid Tumor Tissues by Mass Spectrometry Imaging**; Silvia Giordano<sup>1</sup>; Lavinia Morosi<sup>1</sup>; Roberta Pastorelli<sup>1</sup>; Massimo Zucchetti<sup>1</sup>; Luigi Falciola<sup>2</sup>; Giuseppe Cappelletti<sup>2</sup>; Valentina Pifferi<sup>2</sup>; Melinda Morelli<sup>2</sup>; Sonja Visentin<sup>3</sup>; Enrico Davoli<sup>1</sup>; <sup>1</sup>IRCCS Istituto Mario Negri, Milano, Italy; <sup>2</sup>Chemistry Dept., University of Milan, Milano, Italy; <sup>3</sup>Mol. Biotech. and Health Dept., University of Torino, Torino, Italy
- IMAGING MS: DISEASE MARKERS**  
**668-694**
- TP 668 **Imaging Mass Spectrometry Reveals the Decrease of Cardiolipin on Kidney of NASH Model Mouse**; Takahiro Hayasaka; Hirotohi Fuda; Shu-Ping Hui; Hitoshi Chiba; *Hokkaido University, Sapporo, Japan*
- TP 669 **Using MALDI Mass Spectrometry Imaging to Uncover the Role of Ganglioside Metabolism in Neurodegeneration**; Sarah Caughlin; Kristina Jurcic; Ken Yeung; David Cechetto; Shawn Whitehead; *Western University, London, Canada*
- TP 670 **Functional Metabolic Multimodality Imaging by Dynamic Nuclear Polarization-Magnetic Resonance Imaging and Mass Spectrometry Imaging**; Daisuke Miura; Fuminori Hyodo; Yoshinori Fujimura; *ICMRN, Kyushu University, Fukuoka, Japan*
- TP 671 **MCAEF (Matrix Coating Assisted by an Electric Field): a Novel Technique for Enhanced Imaging of Biomarker Candidates for Prostate Cancer**; Xiaodong Wang<sup>1</sup>; Jun Han<sup>1</sup>; Juncong Yang<sup>1</sup>; Jingxi Pan<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada; <sup>2</sup>Dept. of Biochem. & Microbiol., Univ. of Victoria, Victoria, BC, Canada
- TP 672 **Multimodal Mass Spectrometric Imaging for Targeted Metabolomics of Ovarian Cancer**; Martin R. L. Paine<sup>1</sup>; Rachel V. Bennett<sup>1</sup>; Jaeyeon Kim<sup>2</sup>; L. DeEtte Walker<sup>1</sup>; John McDonald<sup>1</sup>; Martin M. Matzuk<sup>2</sup>; Facundo M. Fernández<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA; <sup>2</sup>Baylor College of Medicine, Houston, TX
- TP 673 **Imaging Mass Spectrometry in Prostate Cancer – Looking Beyond Histology**; Kristina Schwamborn<sup>1,2</sup>; Roopika Menon<sup>3</sup>; Sven Perner<sup>3</sup>; Richard Caprioli<sup>2</sup>; <sup>1</sup>Technical University Munich, Munich, Germany; <sup>2</sup>Vanderbilt University, Nashville, TN; <sup>3</sup>Institute of Pathology, Bonn, Germany
- TP 674 **Histological Examination of FFPE Pancreas Tumor Sections Combined with Imaging Mass Spectrometry Analysis at High Speed and Spatial Resolution**; Jörg Kriegsmann<sup>1,4</sup>; Mark Kriegsmann<sup>2</sup>; Michael Becker<sup>3</sup>; Soeren-Oliver Deininger<sup>3</sup>; Mike Otto<sup>1,4</sup>; Rita Casadonte<sup>4</sup>; <sup>1</sup>Center for Histology, Cytology and Molecular Diagn, Trier, Germany; <sup>2</sup>University of Heidelberg, Heidelberg, Germany; <sup>3</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>4</sup>Proteopath GmbH, Trier, Germany
- TP 675 **Tumor Classification Using Mass Spectrometry and Microarrays**; Jone Garate<sup>1</sup>; Roberto Fernández<sup>1</sup>; Sergio Lage<sup>1</sup>; Arantza Pérez-Valle<sup>2</sup>; Tarson Tolentino-Cortez<sup>2</sup>; Aintzane Asurmendi<sup>1</sup>; Egoitz Astigarraga<sup>2</sup>; María D. Boyano<sup>1</sup>; Gabriel Barreda-Gómez<sup>2</sup>; José A. Fernández<sup>1</sup>; <sup>1</sup>University of Basque Country, Leioa, Spain; <sup>2</sup>IMG Pharma Biotech, Zamudio, Spain
- TP 676 **Imaging Mass Spectrometry of Liver Regeneration after Partial Hepatectomy in Mice Targeting Primary Bile Acids and Nucleotides**; Kohta Iguchi<sup>1</sup>; Yudai Tsuji<sup>2</sup>; Taisuke Nakamura<sup>2</sup>; Tomoyuki Nakamura<sup>3</sup>; Etsuro Hatano<sup>1</sup>; Shinji Uemoto<sup>1</sup>; Masaya Ikegawa<sup>2</sup>; <sup>1</sup>Kyoto University, Kyoto, Japan; <sup>2</sup>Doshisha University, Kyoto, Japan; <sup>3</sup>Kansai Medical University, Hirakata, Japan
- TP 677 **Molecular Imaging of Lipid Alteration and Blood-Brain Barrier Disruption in a Mouse Model of Impact Concussive Traumatic Brain Injury**; Bo Yan<sup>1</sup>; Yi Pu<sup>1</sup>; Andrew M. Fisher<sup>1,2</sup>; Chad A. Tagge<sup>1,2</sup>; Lee E. Goldstein<sup>1,3</sup>; Mark E. McComb<sup>1</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA; <sup>2</sup>College of Engineering, Boston University, Boston, Boston, MA; <sup>3</sup>Boston University Photonics Center, Boston, MA
- TP 678 **3-Dimensional Molecular Imaging of the Optic Chiasm Glioma Microenvironment**; David M. Anderson<sup>1</sup>; Anne Solga<sup>2</sup>; David Gutmann<sup>2</sup>; Shannon Cornett<sup>3</sup>; Kristie Rose<sup>1</sup>; Kevin Schey<sup>1</sup>; Richard Caprioli<sup>1</sup>; <sup>1</sup>Vanderbilt University School of Medicine, Nashville, TN; <sup>2</sup>Washington University School of Medicine, St. Louis, MO; <sup>3</sup>Bruker Daltonics Inc., Billerica, MA
- TP 679 **Identification of Lipid Biomarkers of Human Colon Cancer Using Imaging Mass Spectrometry**; Jone Garate<sup>1</sup>; Joan Bestard-Escalas<sup>2</sup>; Roberto Fernandez<sup>1</sup>; Daniel H. Lopez<sup>2</sup>; Sergio Lage<sup>1</sup>; Rebeca Reigada<sup>2</sup>; Sam Khorrani<sup>2,3</sup>; Jose Reyes<sup>2,4</sup>; Isabel Amengual<sup>2,5</sup>; Gwendolyn Barcelo-Coblijn<sup>2</sup>; Jose A. Fernandez<sup>1</sup>; <sup>1</sup>Universidad del Pais Vasco, Leioa, SPAIN; <sup>2</sup>Research Unit, Hospital

- Universitari Son Espases, Palma, Spain; <sup>3</sup>Gastroenterology Unit, Hospital Universitari Son E, Palma, Spain; <sup>4</sup>Gastroenterology Unit, Hospital Comarcal de Inca, Inca, Spain; <sup>5</sup>Anatomy Unit, Hospital Universitari Son Espases, Palma, Spain*
- TP 680 **Nutrient Sequestration at the Pathogen-Human Host Interface: Imaging Mass Spectrometry reveals Bacterial Subpopulations in Biofilms;** *Jessica Moore<sup>1</sup>; Catherine Wakeman<sup>2</sup>; Michael Noto<sup>2</sup>; Boone Prentice<sup>1</sup>; Jeffrey Spraggins<sup>1</sup>; Michael Becker<sup>3</sup>; Jeremy L. Norris<sup>1</sup>; Eric Skaar<sup>2</sup>; Richard Caprioli<sup>1</sup>; <sup>1</sup>Vanderbilt University MSRC, Nashville, TN; <sup>2</sup>Vanderbilt University School of Medicine, Nashville, TN; <sup>3</sup>Bruker Daltonik GmbH, Bremen, Germany*
- TP 681 **Proteomic Mass Imaging of Pancreas from Type 2 Diabetes (T2D) Rat Model;** *Noriyuki Iwasaki<sup>1</sup>; Kei Masuyama<sup>2</sup>; Hiroshi Wakazono<sup>2</sup>; Takashi Nirasawa<sup>1</sup>; Hirofumi Fujigaya<sup>2</sup>; Masumi Higashiyama<sup>2</sup>; Daisuke Hibi<sup>2</sup>; Mayu Shukutani<sup>3</sup>; Yuki Kuzuhara<sup>3</sup>; Hiroyuki Yanagi<sup>2</sup>; Masaya Ikegawa<sup>3</sup>; <sup>1</sup>Bruker Daltonics K.K., Kanagawa, Japan; <sup>2</sup>Ono Pharmaceutical Co.,Ltd., Osaka, Japan; <sup>3</sup>Doshisha University, Kyoto, Japan*
- TP 682 **A MALDI-MS Imaging Study of Changes in Cardiolipin Distribution in Rat Model of Non-Alcoholic Steatosis;** *Hai-Yan J. Wang<sup>1,2</sup>; Hsuan-Wen Wu<sup>1</sup>; Kuan-Lun Su<sup>1</sup>; Zhi-Fu Zheng<sup>1</sup>; <sup>1</sup>National Sun Yat-Sen University, Kaohsiung, Taiwan; <sup>2</sup>Kaohsiung Medical University, Kaohsiung, Taiwan*
- TP 683 **Visceral Leishmaniasis Biomarkers Discovery by MALDI Imaging Mass Spectrometry;** *Daniele F. O. Rocha<sup>1</sup>; Vanessa G. Santos<sup>1</sup>; Caroline Jaegger<sup>1</sup>; Katia Roberta A. Belaz<sup>1</sup>; Anna Maria A. P. Fernandes A. P. Fernandes<sup>1</sup>; Selma Giorgio<sup>2</sup>; Marcos N. Eberlin<sup>1</sup>; <sup>1</sup>ThoMSon Lab., Chemistry Institute, UNICAMP, Campinas, Brazil; <sup>2</sup>Biology Institute, UNICAMP, Campinas, Brazil*
- TP 684 **MALDI Imaging Mass Spectrometry Reveals Age-Related Deamidation and Truncation of Human Lens Insoluble Proteins;** *Jamie L. Wenke; Kristie L. Rose; Jeffrey Spraggins; Kevin L. Schey; Vanderbilt University, Nashville, TN*
- TP 685 **MALDI-MS Lipid Imaging and [11C] Acetate PET of Tumour Heterogeneity in Non-Small-Cell Lung Cancer;** *Fiona Henderson<sup>1</sup>; David Lewis<sup>2</sup>; Philippa Hart<sup>3</sup>; Kevin Brindle<sup>2</sup>; Dmitry Soloviev<sup>2</sup>; Kaye Williams<sup>1</sup>; Adam McMahon<sup>1</sup>; <sup>1</sup>University of Manchester, Manchester, UK; <sup>2</sup>CRUK-Cambridge Institute, University of Cambridge, Cambridge, UK; <sup>3</sup>Shimadzu, Manchester, UK*
- TP 686 **Large-Scale Mass Spectrometry Imaging Investigation of Cortical Spreading Depression in a Mouse Model of Migraine;** *Ricardo Carreira<sup>1</sup>; Benjamin Balluff<sup>1</sup>; Walid Abdelmoula<sup>1</sup>; Jouke Dijkstra<sup>1</sup>; Michel Ferrari<sup>1</sup>; Else Tolner<sup>1</sup>; Arn van den Maagdenberg<sup>1</sup>; Liam McDonnell<sup>2</sup>; <sup>1</sup>LUMC, Leiden, NL; <sup>2</sup>LUMC & PSF, Pisa, Italy*
- TP 687 **Investigation of Biomarkers of Laser-Induced Retinal Damage Using Mass Spectrometric Imaging;** *Richard F. Reich; Joseph M. Champaign; US Air Force, Usaf Academy, Colorado [CO]*
- TP 688 **Proteomic Imaging of amyloids in Brains from Amyloid Precursor Protein (APP) Transgenic Mice in comparison with Human Alzheimer Amyloid;** *Masaya Ikegawa<sup>1</sup>; Tomohiro Miyasaka<sup>1</sup>; Noriyuki Iwasaki<sup>2</sup>; Takashi Nirasawa<sup>2</sup>; Hiroyuki Sumikura<sup>3</sup>; Shigeo Murayama<sup>3</sup>; Yasuo Ihara<sup>4</sup>; <sup>1</sup>Doshisha University, Kyoto, Japan; <sup>2</sup>Bruker Daltonics K.K., Yokohama, Japan; <sup>3</sup>Tokyo Metropolitan Geriatric Hospital and Inst., Tokyo, Japan; <sup>4</sup>Doshisha University, Graduate School of Brain Scie, Kyoto, Japan*
- TP 689 **Multimodal Imaging of Rat Brain, 1-3 Months Post Stroke: A MALDI MS Insight into Long Term Molecular Expression;** *Philippa Hart<sup>1</sup>; Fiona Henderson<sup>2</sup>; Luis Mancera<sup>1</sup>; Omar Belgacem<sup>1</sup>; Herve Boutin<sup>2</sup>; Adam McMahon<sup>2</sup>; <sup>1</sup>Shimadzu, Manchester, UK; <sup>2</sup>Wolfson*
- Molecular Imaging Centre, Manchester, UK*
- TP 690 **Studies of Diabetic Myocardial Infarction: In Situ Hydrogel-Mediated Protein Digestion Augments the Identification of Protein Changes Detected by MALDI IMS;** *Audra Judd; Salisha Hill; Jeremy L. Norris; Michelle Reyzer; Jeffrey Spraggins; Kristie L. Rose; Michael F. Hill; Richard Caprioli; Vanderbilt University School of Medicine, Nashville, TN*
- TP 691 **Glycopathology Characterization of an N-Glycan Biomarker Panel for Pancreatic Cancer Tissues Using MALDI Imaging Mass Spectrometry and Other Methods;** *Thomas W. Powers<sup>1</sup>; Benjamin A. Neely<sup>1</sup>; Huiyuan Tang<sup>2</sup>; Huarong Xu<sup>1</sup>; Peng Gao<sup>1</sup>; Anand S. Mehta<sup>3</sup>; Brian H. Haab<sup>2</sup>; Richard R. Drake<sup>1</sup>; <sup>1</sup>Medical University of South Carolina, Charleston, SC; <sup>2</sup>Van Andel Institute, Grand Rapids, MI; <sup>3</sup>Drexel University, Doylestown, PA*
- TP 692 **Polarity Switching Mass Spectrometry Imaging of Lipids Using Infrared Matrix-Assisted Laser Desorption Electrospray Ionization (IR-MALDESI) Coupled to a Q-Exactive Plus;** *Milad Nazari; Elias Rosen; David C. Muddiman; North Carolina State University, Raleigh, NC*
- TP 693 **Visualizing Lipid Inflammatory Pathways in Advanced Pulmonary Tuberculosis Lesion Development by MALDI-MSI and Immunohistochemistry;** *Brendan Prideaux; Pei-Yu Chen; Nancy Ruel; Matt Zimmerman; Eliseo Eugenin; Véronique Dartois; PHRI, New Jersey Medical School, Rutgers, Newark, NJ*
- TP 694 **Ion Mobility Mass Spectrometry Imaging of the Human Intraocular Malignancy, Uveal Melanoma;** *Laura M. Cole<sup>1</sup>; Hardeep S Mudhar<sup>2</sup>; Karen Sisley<sup>2</sup>; Malcolm R. Clench<sup>1</sup>; <sup>1</sup>Sheffield Hallam University, Sheffield, UK; <sup>2</sup>Royal Hallamshire Hospital, Sheffield, UK*





7:30 – 8:00 am..... Set up all Wednesday posters  
 10:30 am – 1:00 pm..... Odd-numbered posters present  
 12:00 – 2:30 pm..... Even-numbered posters present  
 7:30 – 8:00 pm..... Remove all Wednesday posters

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Proteins: Conformation Analysis.....	648-658
Antibodies and Antibody: Drug Conjugates I.....	659-687

### ELEMENTAL ANALYSIS: GENERAL 001-022

- WP 001 **A Polar Reversed-Phase UPLC/Ultrahigh-Resolution MS Method for Molecular Profiling and Quantitation of Naphthenic Acids in Oil Sands Process Water;** Jun Han<sup>1</sup>; Karen Lin<sup>1</sup>; Yi Yi<sup>2</sup>; John Gibson<sup>2</sup>; Christoph Borchers<sup>3</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada; <sup>2</sup>Alberta Innovates – Technology Futures, Victoria, BC, Canada; <sup>3</sup>Dept. of Biochem & Microbiol., Univ. of Victoria, Victoria, BC, Canada
- WP 002 **Development of a  $\mu$ -SPE-direct Sample Analysis Mass Spectrometry Method for the Identification and Quantification of Disinfection By-Products;** Lydon Alexandrou<sup>1</sup>; Oliver Jones<sup>1</sup>; Andrew Minett<sup>2</sup>; <sup>1</sup>ACROSS, School of Applied Sciences, RMIT University, Melbourne, VIC, Australia; <sup>2</sup>EPREP Pty Ltd, Mulgrave, VIC, Australia
- WP 003 **Determination of As, Se and Zn in Superalloy by Dynamic Reaction Cell of Inductively Coupled Plasma Mass Spectrometry;** Jingyu Hu; Yanxia Hou; Guowu Yang; Mei Han; Lixia Yang; , Beijing, BEIJING
- WP 004 **High Performance Liquid Chromatography - Mass Spectrometry Identification of Tobacco-Specific Nitrosamines in Drinking Water;** Xing-Fang Li<sup>1</sup>; Beibei Chen<sup>2</sup>; Yichao Qian<sup>1</sup>; <sup>1</sup>University of Alberta, Edmonton, Canada; <sup>2</sup>Wuhan University, Wuhan, CN
- WP 005 **GC/MS Analysis of Volatile Water Pollutants with Rapid On-Site Sample Preparation;** Olga Polyakova<sup>1</sup>; Viatcheslav Artaev<sup>2</sup>; Albert T. Lebedev<sup>1</sup>; <sup>1</sup>Moscow State University, Moscow, Russian Federation; <sup>2</sup>LECO Corporation, St Joseph, MI
- WP 006 **GC-APLI for Trace Analysis of PAHs in Particulate Matter from Ambient Air;** Masha Pitiranggon<sup>1</sup>; Thomas Arthen-Engeland<sup>2</sup>; Verena Tellstroem<sup>2</sup>; Beizhan Yan<sup>1</sup>; Carsten Baessmann<sup>2</sup>; <sup>1</sup>Lamont-Doherty Earth Observatory of Columbia Univ., Palisades, NY; <sup>2</sup>Bruker Daltonik GmbH, Bremen, Germany
- WP 007 **Experimental and Theoretical Insights into H<sub>2</sub>O Activation by Th<sup>+</sup>: The Spin-Orbit Effect;** Richard Cox<sup>1</sup>; Peter Armentrout<sup>2</sup>; <sup>1</sup>Department of Chemistry, University of Utah, Salt Lake City, UT; <sup>2</sup>University of Utah, Salt Lake City, UT
- WP 008 **Development of a Rapid Ion Chromatography-Tandem Mass Spectrometry Method for Simultaneous Analysis of Haloacetic Acids and Related Halogen Compounds;** Runmiao Xue<sup>1,2</sup>; Honglan Shi<sup>1,2</sup>; John Yang<sup>3</sup>; Enos Inniss<sup>4</sup>; <sup>1</sup>Missouri University of Science and Technology, Rolla, MO; <sup>2</sup>Center for CS3M, Rolla, MO; <sup>3</sup>Lincoln University of Missouri, Jefferson City, MO; <sup>4</sup>University of Missouri-Columbia, Columbia, MO
- WP 009 **Fragmentation Trees for Automated *de novo* Interpretation of Impure Electron Ionization Spectra from Gas Chromatographic Complex Mixture Analysis: Chemical Deconvolution;** Kevin Siek<sup>1</sup>; Vasily Makarov<sup>2</sup>; Viatcheslav Artaev<sup>1</sup>; Dmitry Mazur<sup>3</sup>; Albert T. Lebedev<sup>3</sup>; <sup>1</sup>LECO Corporation, Saint Joseph, MI; <sup>2</sup>Mass Spectrometry Consulting Ltd., Bar, Montenegro; <sup>3</sup>Moscow State University, Moscow, Russian Federation
- WP 010 **Novel Approach for *in vivo* Metabolic and Contaminant Profiling of Underwater Ecosystems by LC-HRMS using Solid Phase Microextraction as a Sampling Tool;** Barbara Bojko<sup>1,2</sup>; Ezel Boyaci<sup>1</sup>; Krzysztof Goryński<sup>1,2</sup>; Thanos Dailianis<sup>3</sup>; Evangelina Yiantzi<sup>4</sup>; Eleftheria Psillakis<sup>4</sup>; Janusz Pawliszyn<sup>1</sup>; <sup>1</sup>University of Waterloo, Waterloo, Canada; <sup>2</sup>Collegium Medicum, Nicolaus Copernicus University, Torun, Poland; <sup>3</sup>Hellenic Centre for Marine Research, Heraklion, Crete, Greece; <sup>4</sup>Technical University of Crete, Chania, Greece
- WP 011 **Determination of BMAA, DAB, AEG and Three Alkaloid Cyanotoxins in Lake Water using Dansyl Chloride Derivatization and UHPLC-HESI-HRMS Detection;** Audrey Roy-Lachapelle; Morgan Sollicé; Sébastien Sauvé; <sup>1</sup>Université de Montréal, Montréal, Canada
- WP 012 **Non-targeted Approach for the Evaluation of Concentration Fluctuations in the Effluent of Different Wastewater Treatment Plants;** Matthias Ruff; Rahel Comte; Martin Loos; Heinz Singer; <sup>1</sup>Eawag, Dübendorf, Switzerland
- WP 013 **Thermal Desorption - Gas Chromatography - High Resolution Time-of-Flight Mass Spectrometry (TD-GC- HRT MS) for Analysis of Geochemical Biomarkers;** Giovana Bataglion<sup>1</sup>; Clécio Klitzke<sup>2</sup>; Joe Binkley<sup>2</sup>; Jeffrey Patrick<sup>2</sup>; Marcos Eberlin<sup>1</sup>; <sup>1</sup>Unicamp, Campinas, SP-Brazil; <sup>2</sup>LECO Corporation, St. Joseph, MI
- WP 014 **Detection of Toxic Substances in Environmental Samples by Liquid Chromatography-Tandem Mass Spectrometry and Metabolomics;** Sam Li; Wenlin Zhang; Si Ni Lee; Le Rong; Thawatchai Maneerung; Chi-Hwa Wang; Koon Gee Neoh; <sup>1</sup>National University of Singapore, Singapore, Singapore
- WP 015 **Accurate Mass Quantification of Brominated Flame Retardants in Milk by Q-TOF Based;** Xin Ma; Zheng-xiang Zhang; Tao Bo; <sup>1</sup>Agilent Technologies, Beijing, China



## WEDNESDAY POSTERS

- WP 016 **Screening Lake Trout for Perfluorinated and Polyfluorinated Compounds in Lake Trout Using UPLC-QToF in Mse Mode;** Sadjad Fakouri Baygi; Bernard Crimmins; Thomas Holsen; *Clarkson University, Potsdam, NY*
- WP 017 **The Detection of Trace Organic Pollutes by the Ion-Molecular Reaction of Arylnitrenium Ions in Gas Phase via Mass Spectrometry;** Lei Yue<sup>1</sup>; Chuanfan Ding<sup>2</sup>; Yuanjiang Pan<sup>1</sup>; <sup>1</sup>*Department of chemistry, Zhejiang University, Hang Zhou, China;* <sup>2</sup>*Department of chemistry, Fudan University, Shang Hai, China*
- WP 018 **Method Optimization for the Separation and Quantification of Key Metabolites in Daphnia magna tissues;** Philippe Venne<sup>1</sup>; Viviane Yargeau<sup>2</sup>; Pedro A. Segura<sup>1</sup>; <sup>1</sup>*University of Sherbrooke, Sherbrooke, Canada;* <sup>2</sup>*McGill University, Montreal, Canada*
- WP 019 **Determination of Phthalates in Environmental Matrices;** Oihana Ros Ibarretxe<sup>1</sup>; Grazina Pacepavicius<sup>2</sup>; Tommy Bisbicos<sup>2</sup>; Ailette Prieto Sobrino<sup>1</sup>; Asier Vallejo Ruiz<sup>1</sup>; Mehran Alaei<sup>2</sup>; <sup>1</sup>*University of the Basque Country (UPV/EHU), Bilbao, Spain;* <sup>2</sup>*Environment Canada, Burlington, Canada*
- WP 020 **Uranium Quantification in Ores by Microwave Plasma Torch Tandem Mass Spectrometry;** Meiling Yang; Eric Handberg; Juchao Liang; Huanwen Chen; *East China Institute of Tech., Nanchang, China*
- WP 021 **Orbitrap Mass Spectrometry Characterization of Water Samples Derived from Athabasca Lean Oil Sands and Mixed Surficial Materials;** John Headley<sup>1</sup>; Kerry M. Peru<sup>1</sup>; Chris Swyngedouw<sup>2</sup>; Ian Fleming<sup>3</sup>; <sup>1</sup>*Environment Canada, Saskatoon, Canada;* <sup>2</sup>*Exova, Calgary, Canada;* <sup>3</sup>*University of Saskatchewan, Saskatoon, Canada*
- WP 022 **Soil Humic Acids- A Potential Common Source and Formation Process Elucidated by ESI-FTICR-MS;** Nicole DiDonato; Hongmei Chen; Derek Waggoner; Patrick Hatcher; *Old Dominion University, Norfolk, VA*

### NANOMATERIALS 023-034

- WP 023 **The Evaluation of Amine Core Dendrimers as Calibrants for Electrospray Ionization (ESI) and Matrix-Assisted Laser Desorption/Ionization (MALDI) Mass Spectrometry;** Brittany K. Casey; Scott M. Grayson; *Tulane University, New Orleans, LA*
- WP 024 **Single Particle Inductively Coupled Plasma-Mass Spectrometry Analysis of Nanoparticles Uptake by Crops;** Yongbo Dan<sup>2,3</sup>; Honglan Shi<sup>2</sup>; Xingmao Ma<sup>1,3</sup>; Weilan Zhang<sup>1</sup>; Runmiao Xue<sup>2</sup>; Chady Stephan<sup>4</sup>; <sup>1</sup>*Southern Illinois University, Carbondale, IL;* <sup>2</sup>*Missouri University of Science and Technology, Rolla, MO;* <sup>3</sup>*CS3M center at Missouri University of Sci&Tech, Rolla, MO;* <sup>4</sup>*PerkinElmer Inc, Woodbridge, On*
- WP 025 **Investigation of Substrate-Assisted Laser Desorption for Gold Nanoparticle Analysis with ICP MS;** Iva Benešová<sup>1</sup>; Kristýna Dlabková<sup>1</sup>; Tomáš Vaculovič<sup>1,2</sup>; Viktor Kanický<sup>1,2</sup>; Jan Preisler<sup>1,2</sup>; <sup>1</sup>*Masaryk University, Brno, Czech Republic;* <sup>2</sup>*CEITEC MU, Brno, Czech Republic*
- WP 026 **A Novel Carrier Based on TiO<sub>2</sub> Suitable for Isolation of His-tagged Recombinant Proteins and Peptides;** Rudolf Kupcik; Jan Macak; Pavla Krulisova; Pavel Rehulka; Zuzana Bilkova; *University of Pardubice, Pardubice, Czech Republic*
- WP 027 **Surface Characterization of Nanometer-Thick Organic Layers on Nanomaterials using Ambient Ionization Mass Spectrometry;** Sharanya Reddy; Chady Stephan; Craig Whitehouse; *PerkinElmer, Shelton, CT*
- WP 028 **Enhanced LDI-MS Detection of Gold Nanoparticles in Biological Samples using the Synergy between Added Matrix and the Gold Core;** Alyssa Marsico; Sukru Gokhan Elci; Daniel Moyano; Gulen Yesilbag Tonga; Bradley Duncan; Ryan Landis; Vincent M. Rotello; Richard Vachet; *University of Massachusetts Amherst, Amherst, MA*
- WP 029 **Polypyrrole/Multi-walled Carbon Nanotube Composites Combined with GC-MS/MS for Determination of Ultraviolet Filters and its Metabolites in River Water and Urine;** Yu-Chen Liao; Yu-Min Liu; Maw-Rong Lee; *National Chung-Hsing University, Taichung, Taiwan*
- WP 030 **Solid Matrices for the Small Molecule Analysis using MALDI-TOF Mass Spectrometry;** Jo-Il Kim; Jae-Chul Pyun; *Yonsei University, Seoul, South Korea*
- WP 031 **The Use of Ion Mobility Spectrometry-Mass Spectrometry (IMS-MS) to Elucidate Arm-Dispersion within Star Polymers;** Scott M. Grayson<sup>1</sup>; Casey D. Foley<sup>2</sup>; Boyu Zhang<sup>1</sup>; Sarah Trimpin<sup>2</sup>; <sup>1</sup>*Tulane University, New Orleans, LA;* <sup>2</sup>*Wayne State University, Detroit, MI*
- WP 032 **Quantitative Analysis of Drug Loading on Nanoparticle-based Cancer Therapeutics using Scanning Particle Mobility Mass Spectrometry;** Sherrrie Elzey<sup>1</sup>; De-Hao Tsai<sup>2</sup>; Tae Joon Cho<sup>2</sup>; Julien Gigault<sup>2</sup>; Vincent Hackley<sup>2</sup>; <sup>1</sup>*TSI Incorporated, Shoreview, MN;* <sup>2</sup>*National Institute of Standards and Technology, Gaithersburg, MD*
- WP 033 **Binding Selectivity of Cucurbit[5]uril (CB5) and Substituted Cucurbit[5]uril For Anions in the Gas Phase;** Jiewen Shen; David V. Dearden; *Brigham Young University, Provo, UT*
- WP 034 **9.4 T FT-ICR Mass Spectrometer with Cluster Ion Source for Analysis of Formation and Structure of Metallofullerenes and Other Nanomaterials;** Paul W. Dunk<sup>1,2</sup>; Nathan K. Kaiser<sup>2</sup>; Alan G. Marshall<sup>1,2</sup>; Harold W. Kroto<sup>1</sup>; <sup>1</sup>*Florida State University, Tallahassee, FL;* <sup>2</sup>*National High Magnetic Field Laboratory, Tallahassee, FL*

### ENERGY: BIOFUEL AND MINOR FUEL COMPONENTS 035-047

- WP 035 **Quantification of an Anionic Surfactant in Brine Using Solvent Extraction Followed by Spectrophotometry, Evaporative Light Scattering Detection, and Mass Spectrometry;** Mark Romanczyk; Xueming Dong; Ravikiran Yerabolu; Hilka Kenttamaa; *Purdue University, West Lafayette, IN*
- WP 036 **Chemical Fingerprinting of Fast and Slow Pyrolysis Oils with Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Janne Janis; *University of Eastern Finland, Joensuu, Finland*
- WP 037 **Screening of Ligands as Copper Sequestering Agent by Electrospray Mass Spectrometry (ESI-MS): A Clue for Additivition of Diesel Fuel;** Cécile Perret<sup>1</sup>; Hélène Nierengarten<sup>3</sup>; Amandine Racaud<sup>4</sup>; Géraldine Papin<sup>4</sup>; Aziz Jouaiti<sup>2</sup>; Mir Wais Hosseini<sup>2</sup>; Emmanuelle Leize-Wagner<sup>1</sup>; <sup>1</sup>*LSMIS - UMR 7140 CNRS/University of Strasbourg, Strasbourg, France;* <sup>2</sup>*LTM - UMR 7140 CNRS/University of Strasbourg, Strasbourg, France;* <sup>3</sup>*Service de Spectrométrie de Masse - UMR 7177, Strasbourg, France;* <sup>4</sup>*CReS - TOTAL, Solaize, France*
- WP 038 **Field-portable GC/MS for the Direct Analysis of Fuel Tracers;** Philip Tackett; Cynthia Liu; Leonard Rorrer; Mitch Wells; Dennis Barket, Jr; *FLIR Systems, West Lafayette, IN*
- WP 039 **Structural Effects on the Ionization Response of Lignin Model Compounds during Electrospray Ionization;** Fan Huang; Bert C. Lynn; *University of Kentucky, Lexington, KY*
- WP 040 **Biomarker Identification in Crude Oil by using Gas Chromatography/ High-Resolution Mass Spectrometry with Electron Ionization and Field Ionization;** Masaaki Ubukata; A. John Dane; Robert B. Cody; *JEOL USA, INC., Peabody, MA*
- WP 041 **Thin-film Pyrolysis High Resolution Mass Spectrometry of Glucose-based Carbohydrates: Real-time Monitoring of Products and Their Temporal Profiles;** Daniel Cole; Carolyn Hutchinson; Young Jin Lee; *Iowa State Univ Chemistry Dept, Ames, IA*
- WP 042 **Analysis of Biodiesel Contamination In Jet Fuel using Supercritical Fluid Chromatography-Electrospray Ionisation Mass Spectrometry (SFC-ESI-MS);** Waraporn



- Ratsameepakaj<sup>1</sup>; Julie Herniman<sup>1</sup>; Tim Jenkins<sup>2</sup>; G John Langley<sup>1</sup>; <sup>1</sup>University of Southampton, Southampton, UK; <sup>2</sup>Waters Corporation, Wilmslow, UK
- WP 043 **Molecular Level Characterization of Solid Graphite Pitches by High Resolution MALDI Ion Mobility Mass Spectrometry**; Wen Zhang; Hans Joachim Räder; Klaus Müllen; *MPI for Polymer Research, Mainz, Germany*
- WP 044 **The Carbon Isotopic (<sup>13</sup>C/<sup>12</sup>C) Signature of Sugar Cane Bioethanol: Certifying the Major Source of Renewable Fuel from Brazil**; Laura A. Neves<sup>1</sup>; Gabriel F. Sarmanho<sup>1</sup>; Valnei. S. Cunha<sup>1</sup>; Romeu J. Daroda<sup>1</sup>; Marcos N. Eberlin<sup>2</sup>; Maira Fasciotti<sup>1,2</sup>; <sup>1</sup>INMETRO, Duque De Caxias, Brazil; <sup>2</sup>University of Campinas, UNICAMP, Campinas, Brazil
- WP 045 **Fragmentation of Deprotonated Model Compounds with Lignin – Carbohydrate Linkages upon Collision – Activated Dissociation (CAD)**; Christopher Marcum; Weijuan Tang; Huaming Sheng; Tiffany Jarrell; Hilikka Kenttämää; *Purdue University, West Lafayette, IN*
- WP 046 **Characterization of a Municipal Solid Waste Pyrolysis Oil by Electrospray Ionization FT-ICR Mass Spectrometry**; Rebecca Beasley<sup>1</sup>; Alan G. Marshall<sup>1,2</sup>; Ryan P. Rodgers<sup>1,3</sup>; <sup>1</sup>The Florida State University, Tallahassee, FL; <sup>2</sup>Ion Cyclotron Resonance Prog, Tallahassee, FL; <sup>3</sup>Future Fuels Institute, Tallahassee, FL
- WP 047 **Exploring Mechanisms of Fast Pyrolysis of Lignin via Tandem Mass Spectrometry and Quantum Chemical Calculations: A Synthetic Model Compound Study**; Priya Murria; Jinshan Gao; John C. Degenstein; Huaming Sheng; Matthew R. Hurt; John J. Nash; Hilikka I. Kenttämää; *Purdue University, West Lafayette, U.S.*
- FOOD SAFETY**  
**048-082**
- WP 048 **Improved Analysis of Veterinary Drug Residues in Biological Tissues by UHPLC-MS/MS**; Alan Lightfield; *U.S. Dept. of Agriculture, Wyndmoor, PA*
- WP 049 **Applications of Liquid Chromatography-High Resolution Mass Spectrometry for the Analysis of Pesticides in Fresh Produce and Teas**; Kelli Simon<sup>1</sup>; Jon Wong<sup>1</sup>; Alexander Krynitsky<sup>1</sup>; Zhengwei Jia<sup>2</sup>; Jian Wang<sup>3</sup>; James Wittenberg<sup>1</sup>; Hoon Park<sup>1</sup>; <sup>1</sup>FDA, College Park, MD; <sup>2</sup>Shanghai Institute for Food and Drug Control, Shanghai, China; <sup>3</sup>Canadian Food Inspection Agency, Calgary AB, Canada
- WP 050 **Determination of Pesticides in Foods using Dopant-optimized Gas Chromatography-Atmospheric Pressure Chemical Ionization Quadrupole-Time-of-Flight Mass Spectrometry**; Kyung Hoon Cha<sup>1,2</sup>; Shin-Kwon Kang<sup>2</sup>; Sawyen Ow<sup>2</sup>; Jong Hwa Lee<sup>1</sup>; Jung-Hak Lee<sup>1</sup>; Jeong-Han Kim<sup>1</sup>; Dong-Ho Kim<sup>3</sup>; <sup>1</sup>Seoul National University, Seoul, Korea; <sup>2</sup>Bruker Korea Ltd., Seongnam-Si, Korea; <sup>3</sup>Experimental Research Institute, NAQS, Gimcheon-si, Korea
- WP 051 **The Use of Silica Plate Imprinting for Molecular Trapping Followed by Laser Desorption Ionization Mass Spectrometry**; Diogo Noin De Oliveira; Mônica Ferreira; Rodrigo Catharino; *Innovare Biomarkers Laboratory - UNICAMP, Campinas, Brazil*
- WP 052 **New Analytical Tools to Tackle an Old Problem: Strategies for the Screening and Identification of Mycotoxins in Food by UHPLC/QTOF/MS**; Elisabeth Varga<sup>1</sup>; Emma Rennie<sup>2</sup>; Thomas Glauner<sup>3</sup>; Michael Sulyok<sup>1</sup>; Maria Vandamme<sup>2</sup>; Rudolf Krska<sup>1</sup>; Franz Berthiller<sup>1</sup>; <sup>1</sup>Univ of Natural Resources and Life Sciences, Vienna (BOKU), Austria; <sup>2</sup>Agilent Technologies Inc, Santa Clara, CA; <sup>3</sup>Agilent Technologies Sales&Services GmbH, Waldbronn, Germany
- WP 053 **Fast GC-MS/MS Analysis of Multicomponent Pesticides Residues (360) in Food Matrices using UHPLC Technology**; Hendrik J. Schulte<sup>1</sup>; Hans-Ulrich Baier<sup>1</sup>; Stephane Moreau<sup>1</sup>; Klaus Bolliq<sup>2</sup>; <sup>1</sup>SHIMADZU Europa GmbH, Duisburg, Germany; <sup>2</sup>Shimadzu, Duisburg, N/A
- WP 054 **A Comparative Study of Targeted Screening Method by LC/MS/MS and Un-targeted Screening Method by LC-TOF in Residual Pesticides Analysis**; Zhaoyi Zhan; Jie Xing; Zhe Sun; Zhi Wei Ting; Yin Ling Chew; *Customer Support Centre, Shimadzu (Asia Pacific), Pte Ltd, Singapore*
- WP 055 **Applying 'Fast GC-MS/MS' using Triple Quadrupole Technology to Increase Productivity for Pesticide Residue Analysis in QuEChERS Extracts**; Cristian Cojocariu<sup>1</sup>; Mike Hetmanski<sup>2</sup>; Richard Fussell<sup>2</sup>; Dominic Roberts<sup>1</sup>; Paul Silcock<sup>1</sup>; Sergio Guazzotti<sup>3</sup>; Jason Cole<sup>3</sup>; <sup>1</sup>Thermo Fisher Scientific, Runcorn, UK; <sup>2</sup>Food and Environment Research Agency, York, UK; <sup>3</sup>Thermo Fisher Scientific, Austin, TX
- WP 056 **Quantitative and Qualitative Confirmation of Pesticides in Beet Extract Using High Resolution Accurate Mass (HRAM) Mass Spectrometry**; Charles T. Yang<sup>2</sup>; Dipankar Ghosh<sup>2</sup>; Olaf Scheibner<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- WP 057 **A Sensitive and Repeatable Method for Characterization of Sulfonamides and Trimethoprim in Honey in QuEChERS Extracts with Liquid-Chromatography-Tandem Mass Spectrometry**; Hernando Escobar; Jeffrey H. Dahl; Eddie Medina; Christopher T. Gilles; *Shimadzu Scientific Instruments, Columbia, MD*
- WP 058 **Analysis of QuEChERS Extracts of a Variety of Foods for Pesticide Residues using Automated SPE Coupled to GC/MS/MS and LC/MS/MS**; Mark J. Hayward<sup>1</sup>; Jonathan Ho<sup>2</sup>; Peter Ratsep<sup>2</sup>; Rick Youngblood<sup>1</sup>; Kim Gamble<sup>1</sup>; <sup>1</sup>ITSP Solutions, Hartwell, GA; <sup>2</sup>Shimadzu, Somerset, NJ
- WP 059 **Reducing Matrix Effects in Multi-Residue Pesticide Analysis by Sample Dilution using a Newly Developed Triple Quadrupole MS with Enhanced Sensitivity**; Mark Sartain<sup>1</sup>; Thomas Glauner<sup>2</sup>; Anabel Fandino<sup>1</sup>; Na Pi Parra<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>Agilent Technologies GmbH, Waldbronn, Germany
- WP 060 **Reduced Cost for Pesticides Residues Analysis by GC/MS/MS Using Mini-QuEChERS and an Ultra-Efficient Ionization Source**; Melissa Churley<sup>1</sup>; Joan Stevens<sup>2</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>Agilent Technologies, Wilmington, DE
- WP 061 **Validation of a Method for the Quantitation of Multiple Pyrrolizidine Alkaloids in Herbal Teas and Honey by UHPLC/MS/MS**; Christina Gottert<sup>1</sup>; Melinda Bittner<sup>1</sup>; Franziska Spitzbarth<sup>1</sup>; Angelika Oltmanns<sup>1</sup>; Thomas Glauner<sup>2</sup>; Na Pi Parra<sup>3</sup>; Steve Royce<sup>3</sup>; Guenther Kempe<sup>1</sup>; <sup>1</sup>LUA Saxony, Pharmacologically Active Compounds, Chemnitz, Germany; <sup>2</sup>Agilent Technologies Sales & Services GmbH, Waldbronn, Germany; <sup>3</sup>Agilent Technologies, Inc., Santa Clara, CA
- WP 062 **Pesticides Target Screening with an Atmospheric Pressure Chemical Ionisation GC Coupled to High-Resolution Q-TOF-MS**; Thomas Arthen-Engeland; Petra Decker; Karin Wendt; Oliver Raether; Verena Tellstroem; Carsten Baessmann; *Bruker Daltonik GmbH, Bremen, Germany*
- WP 063 **Development of an MS/HRMS Library for Rapid Quantitation, Confirmation and Dereplication of Marine Toxins using All-Ion High Resolution Tandem Mass Spectrometry (Q-TOF) Coupled to Ultra-High Performance Liquid Chromatography (UHPLC)**; Manoella Sibat<sup>1</sup>; Zita Zendong<sup>1</sup>; Véronique Séchet<sup>1</sup>; Christine Herrenknecht<sup>2</sup>; Zouher Amzil<sup>1</sup>; Philipp Hess<sup>1</sup>; <sup>1</sup>Ifremer, Laboratoire Phycotoxines, Nantes, France; <sup>2</sup>LUNAM, Université de Nantes, Nantes, France
- WP 064 **Examination of Pesticides in Wine, Beer and Their Constituent Products using High-Throughput Techniques to Maximize Extraction & Efficiency**; Patricia Atkins; *Spex Certiprep, Metuchen, NJ*

- WP 065 **Development of an Analytical Method for Screening and Confirmation of Multi-Class Veterinary Drug Residues in Fish by LC-MS/MS;** Junghyun Kim; Hyun-Deok Cho; Won Jae Kang; Unyong Kim; Han Young Eom; Joon Hyuk Suh; Sang Beom Han; *Chung-Ang University, Seoul, South Korea*
- WP 066 **Application of UHPLC and Quadrupole Orbitrap High-Resolution Mass Spectrometer for Determination of 111 Pesticides Residues in Wines;** Niusheng Xu; *Shanghai, China*
- WP 067 **Evaluation of Variable Data Independent Acquisition (vDIA) Approach for Non-target Screening of Veterinary Drug in Animal Feed;** Zhe Zhou; Zheng Jiang; *Thermo Fisher Scientific, Shanghai, China*
- WP 068 **Optimisation and Validation of a Multi-class, Multi-residue Method for Veterinary Drug Confirmation in Animal Derived Food by UHPLC-MS/MS;** David Baker<sup>1</sup>; Neil J Loftus<sup>1</sup>; Laetitia Fages<sup>2</sup>; Eric Capodanno<sup>2</sup>; Mikael Levi<sup>3</sup>; <sup>1</sup>*Shimadzu, Manchester, UK*; <sup>2</sup>*Phytocontrol, Nimes, France*; <sup>3</sup>*Shimadzu France, Marne-La-Vallée, France*
- WP 069 **Identification of Contaminants in Dog Food by LC Time of Flight Mass Spectrometry with Fragment Ion Confirmation;** Sue Dantonio<sup>1</sup>; Lynne Marshall<sup>2</sup>; Tes Ingbritsen<sup>3</sup>; Stephanie Morgenstern<sup>4</sup>; Joni Stevens<sup>5</sup>; <sup>1</sup>*Agilent Technologies, Cedar Creek, TX*; <sup>2</sup>*Agilent Technologies, Toledo, OH*; <sup>3</sup>*Royal Standard Poodles, Staples, MN*; <sup>4</sup>*DePaul University, Chicago, IL*; <sup>5</sup>*Agilent Technologies, Little Falls, DE*
- WP 070 **A Sensitive and Selective LC-MS/MS Detection and Quantitation of Highly Polar Aminoglycosides Antibiotics in Honey Matrix;** Neha Bhasin<sup>1</sup>; Prasanth Joseph<sup>1</sup>; Praveen Sharma<sup>1</sup>; Manoj Pillai<sup>1</sup>; Jianru Stahl-Zeng<sup>2</sup>; <sup>1</sup>*Sciex, 121, Udyog Vihar, Gurgaon, India*; <sup>2</sup>*Sciex, Darmstadt, Germany*
- WP 071 **Trace Analysis of Dioxins and Dioxin-Like PCBs utilizing GC/MS/MS with a New High Efficiency Source;** Jessica Westland; *Agilent Technologies, Wilmington, Delaware*
- WP 072 **Targeted Multi Residue LC-MS/MS Method for Sulfonamides and Nitroimidazoles Antibiotics in Honey with LC-MS/MS;** Neha Bhasin<sup>1</sup>; Prasanth Joseph<sup>1</sup>; Praveen Sharma<sup>1</sup>; Manoj Pillai<sup>1</sup>; Jens Dahlmann<sup>2</sup>; <sup>1</sup>*Sciex, 121, Udyog Vihar, Phase IV, Gurgaon, Haryana, India*; <sup>2</sup>*Sciex, Darmstadt, Germany*
- WP 073 **Method Development for Fake Lamb Meat Detection using LC-MS/MS system;** Lihai Guo; Haiyan Cheng; Wenhai Jin; Huafen Liu; *AB SCIEX, Beijing, China*
- WP 074 **A High Sensitivity LC/MS/MS Method with QuEChERS Sample Pre-treatment for Analysis of Aflatoxins in Peanut Butter Samples;** Yin Ling Chew<sup>1</sup>; Jie Xing<sup>1</sup>; Zhi Wei Ting<sup>1</sup>; Jun Xiang Lee<sup>2</sup>; Zhaoqi Zhan<sup>1</sup>; <sup>1</sup>*Customer Support Centre, Shimadzu (Asia Pacific), Pte Ltd, Singapore*; <sup>2</sup>*School of Physical & Mathematical Sciences, Nanyang Technological University, Singapore*
- WP 075 **Screening for Pesticide Residues in Fruits and Vegetables by GC/Q-TOF with an Exact Mass Library;** Philip L. Wylie; Joni Stevens; Kumi Shiota Ozawa; Joerg Riener; Wen-wen Wang; Jennifer Gushue; *Agilent Technologies, Wilmington, DE*
- WP 076 **Fast Screening, Identification and Quantification of Pesticide Residues in Baby Food using GC Orbitrap MS Technology;** Cristian Cojocariu<sup>1</sup>; Richard J. Fussell<sup>3</sup>; Mike Hetmanski<sup>3</sup>; Dominic Roberts<sup>1</sup>; Jason Cole<sup>2</sup>; Paul Silcock<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, Runcorn, UK*; <sup>2</sup>*Thermo Fisher Scientific, Austin, TX*; <sup>3</sup>*Food and Environment Research Agency, York, UK*
- WP 077 **Multi-residue Analysis of Pesticides in Crude Food Extracts using a Simple Extraction Technique and LC/MS/MS;** Miho Kawashima<sup>1</sup>; Yuka Fujito<sup>2</sup>; Yayoi Ichiki<sup>3</sup>; Miho Sakai<sup>4</sup>; Takashi Ando<sup>4</sup>; Kiyomi Arakawa<sup>2</sup>; Yoshihiro Hayakawa<sup>2</sup>; <sup>1</sup>*Shimadzu Corporation, Tokyo, Japan*; <sup>2</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>3</sup>*Miyazaki Enterprise Promotion Organization, Miyazaki, Japan*; <sup>4</sup>*Miyazaki Agricultural Research Institute, Miyazaki, Japan*
- WP 078 **LC-MS/MS Analysis of Cyanotoxins in Blue-Green Algal Dietary Supplements: Considerations for Method Development;** Whitney L. Stutts; Christine H. Parker; Stacey L. Degrasse; *FDA/CFRAN, College Park, MD*
- WP 079 **A New Approach for Low-Level Quantification of Pesticide Residues in Fruits and Vegetables using a Microflow-LC-ESI-QTRP/Triple TOF-MS;** Bárbara Reichert<sup>1,2</sup>; Ionara Regina Pizzutti<sup>3</sup>; Ijon iHilda Costabeber<sup>4</sup>; Ana Uclés<sup>5</sup>; Sonia Herrera<sup>5</sup>; Amadeo R. Fernández-Alba<sup>5</sup>; Jianru Stahl-Zeng<sup>6</sup>; Ashley Sage<sup>6</sup>; <sup>1</sup>*Department of Food Science and Technology, UFSM, Santa Maria, Brazil*; <sup>2</sup>*CAPES Foundation, Ministry of Education of Brazil, Brasília, Brazil*; <sup>3</sup>*Center of Research and Analysis of Residues and Contaminants, Santa Maria, RS, Brazil*; <sup>4</sup>*Department of Morphology, UFSM, Santa Maria, Brazil*; <sup>5</sup>*University of Almería, Agrifood, Spain*; <sup>6</sup>*AB Sciex, Darmstadt, Germany*
- WP 080 **Fast, Robust and Reliable Method for the Identification and Quantitation of Sildenafil Residue in Honey using LC-MS/MS;** Praveen Kumar Sharma<sup>1</sup>; Neha Bhasin<sup>1</sup>; Prasanth Joseph<sup>1</sup>; Manoj Pillai<sup>1</sup>; Andre Schreiber<sup>2</sup>; <sup>1</sup>*SCIEX, 121, Udyog Vihar, Phase IV, Gurgaon, India*; <sup>2</sup>*SCIEX, Concord, Ontario, Canada*
- WP 081 **Quantitation of 250 Pesticides in the Chinese Traditional Medicines by Ultra-High Performance Liquid Chromatography Tandem Triple Quadrupole and Quadrupole-Time of Flight Mass Spectrometry;** Chang Jiang<sup>1</sup>; Tao Bo<sup>2</sup>; <sup>1</sup>*Chengdu, China*; <sup>2</sup>*NO.3 Wang jing North Road, Bei jing, China*
- WP 082 **Development of Cost Effective and Sensitive Method for the Analysis of Aflatoxin M1 in Milk Samples;** Ajit Dua<sup>1</sup>; Sanjivan Bahman<sup>1</sup>; S.S. Marwaha<sup>1</sup>; Prasanth Joseph<sup>2</sup>; Neha Bhasin<sup>2</sup>; Praveen Sharma<sup>2</sup>; Manoj Pillai<sup>2</sup>; <sup>1</sup>*Punjab Biotechnology incubator, Mohali, Punjab, India*; <sup>2</sup>*Sciex, 121, Udyog Vihar, Phase IV, Gurgaon, Haryana, India*

#### FOOD "OMICS": MS CHARACTERIZATION OF FOOD AND NUTRITIONAL SUPPLEMENTS 083-105

- WP 083 **Analysis of Coffee Flavor Components Employing Gas Chromatography Mass Spectrometry;** Steven B. Foster; Erik R. Flom; Jacob C. Hunt; Billy Nguyen; Daniel X. Pham; Mai N. Vu; Stephanie I. Allred; Emily P. Erdman; Ronald L. Halterman; *University of Oklahoma, Dept. of Chem & Biochem, Norman, OK*
- WP 084 **Internal Standard Optimization for LC-MS/MS Analysis of Green Tea Catechins;** Jessica Murray; Lincoln Shade; Matthew Vergne; *Lipscomb University, Nashville, Tennessee*
- WP 085 **Basmati or Not Basmati? That is the Question;** Gareth Cleland<sup>1</sup>; Adam Ladak<sup>2</sup>; Steven Lai<sup>2</sup>; Ron Stemmler<sup>2</sup>; Jennifer Burgess<sup>1</sup>; <sup>1</sup>*Waters Corporation, Milford, MA*; <sup>2</sup>*Waters Corporation, Beverly, MA*
- WP 086 **Determination of Meat Authenticity using Peptide Biomarkers and High-Resolution Mass Spectrometry;** Alberto Ruiz<sup>1</sup>; Erik Husby<sup>2</sup>; Dipankar Ghosh<sup>2</sup>; Francis Beaudry<sup>1</sup>; <sup>1</sup>*Université de Montréal, St-Hyacinthe, Canada*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*
- WP 087 **Rapid Direct-injection Analysis of Alkaloids in Tobacco Leaves Using Ultra-High Resolution FT-ICR MS;** Qingxia Zhen<sup>1</sup>; Qing Zhang<sup>2</sup>; Keyu Zhou<sup>2</sup>; Kefei Wang<sup>2</sup>; <sup>1</sup>*Institute of Tobacco, Zhengzhou, Henan, China*; <sup>2</sup>*Bruker Daltonics, Shanghai, China*
- WP 088 **MALDI-TOF MS Analysis of the Enrichment of Peptides Derived from Egg Yolk Phostvitin Using Affinity Microchromatography Techniques;** Sean Doering<sup>1</sup>;



- Michael Thomas<sup>1</sup>; Cindy Vang<sup>2</sup>; Jen Grant<sup>3</sup>; Eun Joo Lee<sup>4</sup>; <sup>1</sup>UW-Stout Applied Science Program, Menomonie, WI; <sup>2</sup>UW-Stout Food Science and Technology Program, Menomonie, WI; <sup>3</sup>Dept. of Biology, Univ. Wisconsin-Stout, Menomonie, WI; <sup>4</sup>Dept. of Food & Nutrition, Univ. Wisconsin-Stout, Menomonie, WI
- WP 089 **Non-target Metabolomic Approach for Study of the Dynamic Chemical Changes and Flavor of Black Tea during Fermentation Processing**; Junfeng Tan<sup>1</sup>; Weidong Dai<sup>1</sup>; Meiling Lu<sup>2</sup>; Haipeng Lv<sup>1</sup>; Qunhua Peng<sup>1</sup>; Yue Zhang<sup>1</sup>; Yin Zhu<sup>1</sup>; Zhi Lin<sup>1</sup>; <sup>1</sup>Tea Research Institute, CAAS, Hangzhou, China; <sup>2</sup>Agilent Technologies (China) Limited, Beijing, China
- WP 090 **Authentication of Closely Related Flatfish using Tandem Mass Spectrometry and Spectral Library Matching**; Merel Nessen<sup>1</sup>; Dennis van der Zwaan<sup>1</sup>; Sander Grevers<sup>2</sup>; Hans Dalebout<sup>2</sup>; Martijn Staats<sup>1</sup>; Esther Kok<sup>1</sup>; Magnus Palmblad<sup>2</sup>; <sup>1</sup>RIKILT Wageningen UR, Wageningen, Netherlands; <sup>2</sup>Leiden University Medical Center, Leiden, Netherlands
- WP 091 **Evaluation of Tocopherol Oxidation Products in Edible Oils by DART-QTOF**; Susan Seegers; Bunge North America, Bradley, IL
- WP 092 **Simultaneous Analysis of 15 Water-Soluble Vitamins in Beverages and Dietary Supplements with Multi-Mode ODS Column using LC-MS/MS**; Keiko Matsumoto<sup>1</sup>; Ayano Kakitani<sup>2</sup>; Tomonori Inoue<sup>2</sup>; Jun Watanabe<sup>1</sup>; Itaru Yazawa<sup>3</sup>; Yasushi Nagatomi<sup>2</sup>; Naoki Mochizuki<sup>2</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>Asahi Group Holdings, Limited, Moriya, Japan; <sup>3</sup>Imtakt Corporation, Kyoto, Japan
- WP 093 **Innovative Analytical Approach Based on  $\mu$ -SPE Extraction Combined with UHPLC-PDA Analysis for Quantification of Polyphenols in Different Teas**; Priscilla Porto-Figueira<sup>1</sup>; Jose Figueira<sup>1</sup>; Jorge Pereira<sup>1</sup>; Andrew Minett<sup>3</sup>; Peter Dawes<sup>3</sup>; José Câmara<sup>1,2</sup>; <sup>1</sup>Campus Universitário da Penteada, Funchal, Portugal; <sup>2</sup>Universidade da Madeira, Funchal, Portugal; <sup>3</sup>EPREP, Melbourne, Australia
- WP 094 **Characterisation of Bioactive Cranberry Fractions by Mass Spectrometry**; Marie-Claude Denis; University of Montreal, Montreal, Canada
- WP 095 **Study of Olive Oil Cultivars using LC-MS and Statistical Analysis**; Robert J. Seward; Catherine Stacey; PerkinElmer, Waltham, MA
- WP 096 **An UltraFast Online SPE-MS High Throughput Workflow for Class Prediction in Agricultural and Food Products**; Daniel Cuthbertson<sup>1</sup>; Michelle Romm<sup>2</sup>; <sup>1</sup>Agilent Technologies, Denver, CO; <sup>2</sup>Agilent Technologies, Inc., Wakefield, MA
- WP 097 **An HPLC-MS/MS Method for Separating and Measuring Isobaric Apocarotenoids in Plant Foods and Carotenoid Supplements**; Ken Riedl; Jessica Cooperstone; Bolu Durojaye; Earl Harrison; Robert Curley Jr; Steven Schwartz; The Ohio State University, Columbus, OH
- WP 098 **Dry Beans Pre-soak Preparation Methods: What Information Does ESI-MS Provide from Direct Sample Analysis?** Stephen F. Macha; Larry Sallans; University of Cincinnati, Cincinnati, OH
- WP 099 **Cooked Meat Product Analysis by LCMS/MS to Determine between Animal Species using Proteotypic Peptide Quantitative Proteomic Analysis**; Alan Barnes<sup>1</sup>; Neil J Loftus<sup>1</sup>; Junko Iida<sup>2</sup>; <sup>1</sup>Shimadzu MS/BU, Manchester, UK; <sup>2</sup>Shimadzu, Kyoto, Japan
- WP 100 **Fast Amino Acid Analysis of Food Products Using a Novel LCMS System**; Steven M. Wishnies; Shimadzu Scientific, Columbia, MD
- WP 101 **Analysis of Volatile and Semi-Volatile Compounds in Ground Black Pepper by Solid Probe-GC/QTOF with Novel High Efficiency EI Source**; Jennifer Sanderson; Agilent Technologies, Santa Clara, CA
- WP 102 **The Applicability of MALDI-MS to High-throughput Metabolic Profiling of Diverse Green Tea Extracts with Antioxidant Activity**; Yoshinori Fujimura; Asako Nakamura; Daichi Yukihira; Rie Nishimuta; Eisuke Hayakawa; Daisuke Miura; Hirofumi Tachibana; Hiroyuki Wariishi; ICMRN, Kyushu University, Fukuoka, Japan
- WP 103 **LC-MS/MS Analysis of the New Antioxidant Identified from a Soft-Body Extract of Crassostrea gigas**; Mitsugu Watanabe<sup>1</sup>; Kazuyo Fukushima<sup>1</sup>; Jun Watanabe<sup>2</sup>; <sup>1</sup>Watanabe Oyster Laboratory Co., Ltd., Hachioji, Japan; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan
- WP 104 **Determination of Amino Acids using a Novel Liquid Chromatography Compact Mass Spectrometry System (LC-CMS) with Ion Exchange Separation Media**; Daniel Eikel; Simon J. Prosser; Jack D. Henion; Advion Inc., Ithaca, NY
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- WP 181 **G-quadruplex Turncoats: An IMS-MS Investigation of Cation-Dependent Folding and Stability of G-quadruplex-DNA Double Switches;** Eric Largy<sup>1,2</sup>; Adrien Marchand<sup>1,2</sup>; Jean-Louis Mergny<sup>1,2</sup>; Valerie Gabelica<sup>1,2</sup>; <sup>1</sup>*University of Bordeaux, IECB, Pessac, France*; <sup>2</sup>*INSERM, U869, ARNA Laboratory, Bordeaux, France*
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- WP 183 **Development of Facile Pretreatment Method Using Home-Made Pretreatment Device for LC-MS/MS Analysis of Trace Amounts of DNA Adducts;** Hiroya Murakami<sup>1</sup>; Rieko Kawamura<sup>2</sup>; Bunji Uno<sup>2</sup>; Norio Teshima<sup>1</sup>; Yasushi Ishihama<sup>3</sup>; Yukihiko Esaka<sup>2</sup>; <sup>1</sup>*Aichi Institute of Technology, Toyota, Japan*; <sup>2</sup>*Gifu Pharmaceutical University, Gifu, Japan*; <sup>3</sup>*Kyoto University, Kyoto, Japan*

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- WP 185 **Global and Specific Responses of the Histone Acetylome to Systematic Perturbation;** Christian Feller<sup>1,2</sup>; Ignasi Forné Ferrer<sup>1,2</sup>; Axel Imhof<sup>1,2</sup>; Peter B. Becker<sup>1,2</sup>; <sup>1</sup>*Adolf-Butenandt-Institute, LMU University, Munich, Germany*; <sup>2</sup>*Center for Integrated Protein Science, Munich, Germany*
- WP 186 **Epigenetic Evaluation of Short-term Cultured Primary Acute Myeloid Leukemia (AML) Cells Survival Using Mass Spectrometry Based Quantitative Proteomics;** Özlem Önder; Simone Sidoli; Martin Carroll; Benjamin A. Garcia; *University of Pennsylvania, Philadelphia, PA*
- WP 187 **Slicing Through the Complexity of Histone Post Translation Modifications Using High Resolution / Accurate Mass Data Independent Acquisition;** Michael Blank<sup>1</sup>; Simone Sidoli<sup>2</sup>; Andreas FR Huhmer<sup>1</sup>; Benjamin Garcia<sup>2</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*University of Pennsylvania, Philadelphia, PA*
- WP 188 **Characterization of Histone Post-Translational Modifications in the Pathogenesis of Diabetic Retinopathy and Treatment of Minocycline;** Xiaolu Zhao<sup>1</sup>; Simone Sidoli<sup>2</sup>; Wenjun Wang<sup>1</sup>; Leilei Wang<sup>1</sup>; Ole Noerregaard Jensen<sup>2</sup>; Lin Guo<sup>1</sup>; Ling Zheng<sup>1</sup>; <sup>1</sup>*College of Life Science, Wuhan University, Wuhan, P.R.China*; <sup>2</sup>*University of Southern Denmark, Odense, Denmark*
- WP 189 **Relative Quantification of Histone Post Translational Modifications in Time Course Treated MEL Cells using HDAC Inhibitors;** Annie Moradian<sup>1</sup>; Matthias Rädle<sup>2</sup>; Michael J Sweredoski<sup>1</sup>; Sonja Hess<sup>1</sup>; <sup>1</sup>*California Institute of Technology, Pasadena, CA*; <sup>2</sup>*University of Weihenstephan-Triesdorf, Freising, Germany*
- WP 190 **Top-to-bottom MS Characterization of Histone H1 in Breast Cancer Cell Progression;** Michael E. Hoover<sup>1</sup>; Yu Chen<sup>2</sup>; Bettina Sarg<sup>3</sup>; Xibei Dang<sup>2</sup>; Alan A. Shomo<sup>2</sup>; Xiaoyan Guan<sup>2</sup>; Alan G. Marshall<sup>2</sup>; Michael A. Freitas<sup>1</sup>; Herbert Lindner<sup>3</sup>; Nicolas L. Young<sup>2</sup>; <sup>1</sup>*Ohio State University, Columbus, OH*; <sup>2</sup>*National High Magnetic Field Laboratory, Tallahassee, FL*; <sup>3</sup>*Innsbruck Medical University, Innsbruck, Austria*
- WP 191 **Analysis of Differential Epigenetic Histone Marks in 2D-, 3D-cell Culture and Tumor Xenografts;** Tobias Maile<sup>1</sup>; Richard M. Neve<sup>1</sup>; Benjamin Garcia<sup>2</sup>; David Arnott<sup>1</sup>; <sup>1</sup>*Genentech, Inc., S. San Francisco, CA*; <sup>2</sup>*University of Pennsylvania, Philadelphia, PA*
- WP 192 **A Nanoflow LC-MS/MS Approach to Monitor Rapid Loss of 5mC and 5hmC from Differentiating Erythroid Progenitor Genomes;** Scott A. Shaffer; Hien Nguyen; Aishwarya Swaminathan; Daniel Hidalgo; Merav Socolovsky; *University of Massachusetts Medical School,*



- Worcester, MA
- WP 193 **Data-Dependent Analyses of Intact Histone Proteins using Sequential Ion/Ion Reactions and Multiple Fragment Ion Fills on a Chromatographic Time-Scale;** Lissa C. Anderson<sup>1</sup>; Jeffrey Shabanowitz<sup>1</sup>; Kelly R. Karch<sup>2</sup>; Scott A. Ugrin<sup>1</sup>; A. Michelle English<sup>3</sup>; Benjamin A. Garcia<sup>2</sup>; Donald F. Hunt<sup>1</sup>; <sup>1</sup>University of Virginia, Charlottesville, VA; <sup>2</sup>University of Pennsylvania, Philadelphia, PA; <sup>3</sup>Pfizer, Andover, MA
- WP 194 **Linking Epigenetic Regulatory Components with a Chemoresistant Phenotype;** Juan Chavez<sup>1</sup>; Devin Schweppe<sup>1</sup>; Jimmy Eng<sup>1</sup>; Chunxiang Zheng<sup>1</sup>; Alex Taipale<sup>1</sup>; Yiyi Zhang<sup>1</sup>; Kohji Takara<sup>2</sup>; James Bruce<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Himeji Dokkoyo University, Himeji, Japan
- WP 195 **Quantification of Histone Modifications by PRM, a Method Validation;** James Sowers<sup>1</sup>; Hui Tang<sup>1</sup>; In Young Park<sup>2</sup>; Chery Walker<sup>2</sup>; Lawrence Sowers<sup>1</sup>; Kangling Zhang<sup>1</sup>; <sup>1</sup>University of Texas Medical Branch at Galveston, Galveston, TX; <sup>2</sup>Institute of Biosciences and Technology, Texas A&M, Houston, TX
- WP 196 **High Sensitivity Histone Posttranslational Modification Analysis by Preparative SDS-PAGE, with On-Membrane Chemical Derivatization and Tryptic Digestion;** Tommy K. Cheung; Tobias Maile; Marie Classon; David Arnott; Genentech, Inc., South San Francisco, CA
- WP 197 **The Epitranscriptomics of Long Noncoding RNAs in *S. cerevisiae*;** Rebecca E. Rose<sup>1</sup>; Ben Bayly<sup>1</sup>; M.J. Curcio<sup>2</sup>; Daniele Fabris<sup>1</sup>; <sup>1</sup>The RNA Institute, University at Albany, Albany, NY; <sup>2</sup>Wadsworth Center, Albany, NY
- WP 198 **Automated Annotation of Histone Acetylation and Methylation Proteoforms;** Michael J Sweredoski; Annie Moradian; Sonja Hess; California Institute of Technology, Pasadena, CA
- WP 199 **Interplay of Histones and HDAC11 in the Regulation of Human Skeletal Myogenic Differentiation *in vitro*;** Natarajan Bhanu; Benjamin Garcia; University of Pennsylvania, Philadelphia, PA
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- WP 200 **Hydrogel Micropatch Sampling and Mass Spectrometry Provide Insights on Psoriasis Pathophysiology;** Ewelina Dutkiewicz<sup>1</sup>; Kai-Ta Hsieh<sup>1</sup>; Yi-Sheng Wang<sup>2</sup>; Hisen-Yi Chiu<sup>3</sup>; Pawel Urban<sup>1</sup>; <sup>1</sup>Department of Applied Chemistry, NCTU, Hsinchu, Taiwan; <sup>2</sup>Genomics Research Center, Academia Sinica, Taipei, Taiwan; <sup>3</sup>Department of Dermatology, NTU, Taipei, Hsinchu, Taiwan
- WP 201 **Rapid, Comprehensive and Simultaneous Determination of Inborn Errors of Metabolism using a Clinically Validated Untargeted Metabolomics Methodology;** Luke Miller; Anne Evans; Adam Kennedy; Douglas Toal; Metabolan, Inc., Durham, NC
- WP 202 **Ion Pair Chromatography HRAMS Analysis of Positively Charged Metabolites in Fed and Fasting Human Plasma;** Matt Blatnik; John Meissen; Rick Steenwyk; Pfizer Inc., Groton, CT
- WP 203 **Untargeted Ion Mobility-Mass Spectrometry (IM-MS) Based Metabolomics Study of Amniotic Fluid for Preterm Birth with Liquid and Supercritical Fluid Chromatography;** Rafael Montenegro Burke<sup>1</sup>; Maria Hallingstrom<sup>2</sup>; Lisa M. Rogers<sup>3</sup>; Bo Jacobsson<sup>2</sup>; Marian Kacerovsky<sup>4</sup>; David M. Aronoff<sup>3</sup>; John A. Mclean<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>University Hospital East, Goteborg, Sweden; <sup>3</sup>Vanderbilt University Medical Center, Nashville, TN; <sup>4</sup>University Hospital Hradec Kralove, Hradec Kralove, Czech Republic
- WP 204 **HILIC-MS for Metabolomic Profiling: Reveals Potential Insights into Racial Disparity in Prostate Cancer;** Jie Gohlke; Nagireddy Putluri; Arun Sreekumar; Baylor College of Medicine, Houston, TX
- WP 205 **A Metabolomics Study on Heat Stress in Mouse with UHPLC Tandem Quadrupole-Time of Flight Mass Spectrometry;** Wei Du; Tao Bo; Agilent Technologies(China) Co. Ltd., Beijing, China
- WP 206 **Integration of Two Complementary HILIC-TOF MS Methods for Screening Metabolites from Biological Samples in a Metabolomics Service Core Environment;** Li Zhang<sup>1</sup>; Stefaine Wernisch<sup>2</sup>; John Chellman<sup>3</sup>; Manisha Tomar<sup>3</sup>; Jaeman Byun<sup>2</sup>; Subramaniam Pennathur<sup>2</sup>; Charles Burant<sup>1</sup>; <sup>1</sup>The Michigan Regional Comprehensive Metabolomics R, Ann Arbor, MI; <sup>2</sup>University of Michigan, Dept of Internal Medicine, Ann Arbor, MI; <sup>3</sup>EMD Millipore Corporation, Billerica, MA
- WP 207 **Metabolomic Analysis of Melanoma Skin Lesions and Mammalian Cell Cultures by Mass Spectrometry;** Michael T. Costanzo; Candice Z. Ulmer; Matthew S. Kazaleh; Nikolaus Gravenstein; Richard A. Yost; University of Florida, Gainesville, FL
- WP 208 **Discovery of Novel Urinary Galabiosylceramide-Related Biomarkers for Fabry Disease Using a Q-ToF Mass Spectrometry Metabolomic Approach;** Michel Boutin; Christiane Auray-Blais; CHUS-Fleurimont, Sherbrooke, Canada
- WP 209 **Metabolic Signature Profiling as a Diagnostic and Prognostic Tool in Pediatric *Plasmodium falciparum* Malaria;** Izabella Surowiec<sup>1</sup>; Judy Orikiiriza<sup>2</sup>; Elisabeth Karlsson<sup>5</sup>; Mari Bonde<sup>5</sup>; Maria Nelson<sup>5</sup>; Patrick Kyamanwa<sup>3</sup>; Ben Karenzi<sup>4</sup>; Sven Bergström<sup>5</sup>; Johan Trygg<sup>1</sup>; Johan Normark<sup>5</sup>; <sup>1</sup>Department of Chemistry, Umeå University, Umeå, Sweden; <sup>2</sup>Makerere University, Kampala, Uganda; <sup>3</sup>University of Rwanda, Butare, Rwanda; <sup>4</sup>Rwanda Military Hospital, Kigali, Rwanda; <sup>5</sup>Department of Molecular Biology, Umeå University, Umeå, Sweden
- WP 210 **Development of a Liquid Chromatography Quadrupole Time-of-Flight Mass Spectrometry Based Method for the Routine Analysis of Lipids from Plasma Samples;** Linda Ahonen; Anette Untermann; Matej Ore šič; Tuulia Hyötyläinen; Steno Diabetes Center, Gentofte, Denmark
- WP 211 **Qualitative Metabolomics Analysis of Cerebral Spinal Fluid (CSF) in Aneurysmal Subarachnoid Hemorrhage (SAH) Patients;** Tumpa Dutta<sup>1</sup>; William David Freeman<sup>2</sup>; Christian Burrell<sup>2</sup>; Nicole Avalon<sup>2</sup>; Kelly Hines<sup>1</sup>; Godfrey C. (G Charles) Ford<sup>1</sup>; Xuan-Mai T. (Mai) Persson<sup>1</sup>; Mayo Clininc Foundation, Rochester, Rochester, MN; Mayo Clinic, Jacksonville, FL
- WP 212 **High Throughput Liquid Extraction Surface Analysis and Direct Infusion Mass Spectrometric Approaches for Human Urine Global Metabolomics;** Salah Abdelrazig; Catherine Ortori; David Barrett; University of Nottingham, Nottingham, UK
- WP 213 **Exploratory Urinary Metabolomics Study of Type 1 Leprosy Reactions in Nepal;** Oleg A. Mayboroda<sup>1</sup>; Saraswoti Khadge<sup>2</sup>; Susan J.F. van den Eeden<sup>1</sup>; Deanna A. Hagge<sup>2</sup>; Matthias Szesny<sup>3</sup>; Aiko Barsch<sup>3</sup>; Annemieke Geluk<sup>1</sup>; <sup>1</sup>Leiden University Medical Center, Leiden, The Netherlands; <sup>2</sup>Anandaban Hospital, Kathmandu, Nepal; <sup>3</sup>Bruker Daltonics, Bremen, Germany
- WP 214 **Identification and Characterization of Oxygenated Porphobilinogen Derivatives and Their Amino Acid/Peptide Conjugates using Liquid Chromatography-Accurate Mass Tandem Mass Spectrometry;** Christopher Benton; Agilent Technologies, Cheadle, UK
- WP 215 **Application of the Endocrine Metabolites and Nutrition Metabolites Testing in Health Management;** Jiaping Song; Haitao Jia; Song Chen; Fang Li; Hua Li; Aimei Xie; Liangtao Zhang; Liping Lan; Vince Gao; BGI shenzhen, Shenzhen, China
- WP 216 **Epithelial Ovarian Carcinoma Analysis by DESI-MS;** Luisa Doria<sup>1</sup>; Sabine Guenther<sup>2</sup>; Abigail Speller<sup>1</sup>; Anna

- Mroz<sup>1</sup>; Kirill Veselkov<sup>1</sup>; Zoltan Takats<sup>3</sup>; <sup>1</sup>Imperial College of London, London, UK; <sup>2</sup>Imperial College London, Ehringshausen-Kölschhausen; <sup>3</sup>Imperial College London, London
- WP 217 **Integration of Genomics, Proteomics and Lipidomics for Biomarker Discovery of Esophageal Squamous Cell Carcinoma**; Guixue Hou<sup>1,2</sup>; Jin Zi<sup>2</sup>; Liang Lin<sup>2</sup>; Hui Ye<sup>2</sup>; Quanhui Wang<sup>1</sup>; Xiaomin Lou<sup>1</sup>; Lin Wu<sup>1</sup>; Siqi Liu<sup>1,2</sup>; <sup>1</sup>Beijing Institute of Genomics, CAS, Beijing, China; <sup>2</sup>BGI-Shenzhen, Shenzhen, China
- WP 218 **Lipidomics of Nonalcoholic Fatty Liver Disease and Nonalcoholic Steatohepatitis in a Mouse Model via LC-HRMS**; Rainey Patterson<sup>1</sup>; Srilaxmi Kalavalapalli<sup>2</sup>; Nishanth E. Sunny<sup>2</sup>; Timothy Garrett<sup>2</sup>; Richard A. Yost<sup>1,2</sup>; <sup>1</sup>Department of Chemistry, University of Florida, Gainesville, FL; <sup>2</sup>College of Medicine, University of Florida, Gainesville, FL
- WP 219 **Metabolomics of Eye Fluids from Retinoblastoma Patients and Its Correlation to Tissue Gene Expression Studies**; Syed Lateef<sup>1</sup>; Seetaramanjanyulu Gundimeda<sup>1</sup>; Nilanjan Guha<sup>1</sup>; Deepak SA<sup>1</sup>; Arunkumar Padmanaban<sup>1</sup>; Ashwin Mallipatna<sup>2</sup>; Arkasubhra Ghosh<sup>2</sup>; <sup>1</sup>Agilent Technologies, Bangalore, India; <sup>2</sup>GROW Research Lab, Narayana Nethralaya Foundation, Bangalore, India
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- WP 220 **Towards a Comprehensive Characterization of Colorectal Cancer-Associated Glycosylation Changes by Mass Spectrometry**; Stephanie Holst; LUMC, Center for Proteomics and Metabolomics, Leiden, NL
- WP 221 **Sodium Cation Influence on the Salt Bridge Interactions Stabilizing Anionic Arginine/Hexose-Phosphate Complexes**; Ekaterina Darii<sup>1</sup>; Sandra Alves<sup>2</sup>; Alain Perret<sup>1</sup>; Jean-Claude Tabet<sup>2</sup>; <sup>1</sup>CEA-Genoscope/UMR8030, Evry, France; <sup>2</sup>UPMC-IPCM/CSOB/UMR8232, Paris, France
- WP 222 **Determination of Hexuronic acid Stereochemistry in Heparin and Heparan Sulfates Glycosaminoglycans Using Electron Detachment Dissociation**; Isaac Agyekum<sup>1</sup>; Chengli Zong<sup>2</sup>; Geert-Jan Boons<sup>2</sup>; Lingyun Li<sup>3</sup>; Robert J. Linhardt<sup>3</sup>; Jon Amster<sup>1</sup>; <sup>1</sup>University of Georgia, Chemistry Department, Athens, GA; <sup>2</sup>University of Georgia, CCRC, Athens, GA; <sup>3</sup>Rensselaer Polytechnic University, Troy, NY
- WP 223 **Automated Annotation and Identification of Tandem Mass Spectra of Heparin and Heparan Sulfate Oligomers Using a Genetic Algorithm**; Jiana Duan; Jon Amster; University of Georgia, Athens, GA
- WP 224 **A Statistical Model to Estimate the Accuracy of Glycosaminoglycan Identification Made by MS/MS and Database Search**; Yulun Chiu<sup>1</sup>; Paul Schliekelman<sup>2</sup>; Ron Orlando<sup>1</sup>; Joshua S. Sharp<sup>1</sup>; <sup>1</sup>CCRC, University of Georgia, Athens, GA; <sup>2</sup>Department of Statistics, University of Georgia, Athens, GA
- WP 225 **Oligosaccharide Profiling of a NIST Standard Reference Material for Human Milk (SRM 1954) using LC-MS and Spectral Matching**; M. Lorna De Leoz; Stephen Stein; National Institute of Standards & Technology, NIST, Gaithersburg, MD
- WP 226 **Study of N-linked Glycosylation in Different Life Stages of the Red Flour Beetle (*Tribolium castaneum*)**; Nicolas Smargiasso<sup>1</sup>; Tomasz Walski<sup>2</sup>; Els, J. M. Van Damme<sup>2</sup>; Edwin De Pauw<sup>1</sup>; Guy Smaghe<sup>2</sup>; <sup>1</sup>University of Liege, Liege, Belgium; <sup>2</sup>Ghent University, Ghent, Belgium
- WP 227 **Towards de novo Oligosaccharide Sequencing**; Gabe Nagy; Bloomington, IN
- WP 228 **Metabolomics Applied to Ancient Plant Gums in Artworks**; Clara Granzotto<sup>1,2</sup>; Julie Arslanoglu<sup>3</sup>; Christian Rolando<sup>1</sup>; Caroline Tokarski<sup>1</sup>; <sup>1</sup>Université Lille 1, Villeneuve d'Ascq, France; <sup>2</sup>Ca' Foscari University, Venice, Italy; <sup>3</sup>Metropolitan Museum of Art, New York, NY
- WP 229 **HILIC-MS-MS/MS Glycomics Method Development and Application to a Pilot PML Study**; Xiaoping L. Hronowski<sup>1</sup>; Tatiana Plavina<sup>1</sup>; Peter Juhasz<sup>2</sup>; <sup>1</sup>Biogen, Inc., Cambridge, MA; <sup>2</sup>BiogenIdec, Cambridge, MA
- WP 230 **Comprehensive Quantitative and Structural Analysis of Permethylated N-glycan using PGC-LC-MS/MS**; Shiyue Zhou; Xue Dong; Yunli Hu; Yehia Mechref; Texas Tech University, Lubbock, TX
- WP 231 **Evaluating Metabolic and Enzymatic Engineering of a Trastuzumab Mutant Incorporating SiaNAz in CHO Cells**; Edward Bodnar<sup>1</sup>; Celine Raymond<sup>2</sup>; Yves Durocher<sup>2</sup>; Helene Perreault<sup>1</sup>; <sup>1</sup>University of Manitoba, Winnipeg, MB; <sup>2</sup>National Research Council of Canada, Montreal, QC
- WP 232 **Collision-Induced Dissociation of Metalated Carbohydrates and their Electron Transfer Products: Novel Opportunities for Isomer Distinction**; Yuting Huang<sup>1</sup>; Eric D. Dodds<sup>2</sup>; <sup>1</sup>University of Nebraska-Lincoln, Lincoln, NE; <sup>2</sup>University of Nebraska - Lincoln, Lincoln, NE
- WP 233 **Direct Beverage Analysis by SAWN MS**; David Goodlett<sup>1</sup>; Sung Hwan Yoon<sup>1</sup>; Benjamin Oyler<sup>1</sup>; David Kilgour<sup>1</sup>; <sup>1</sup>University of Maryland, Baltimore, MD
- WP 234 **Photon-activation Tandem Mass Spectrometry at Extreme Photon Energy Provides Unprecedented Structural Information on Complex Carbohydrates**; David Ropartz<sup>1</sup>; Alexandre Giuliani<sup>2,3</sup>; Hélène Rogniaux<sup>1</sup>; <sup>1</sup>INRA, UR1268 Biopolymers Interactions Assemblies, Nantes, France; <sup>2</sup>Synchrotron SOLEIL, Gif-sur-Yvette, France; <sup>3</sup>UAR 1008 CEPIA, INRA, Nantes, France
- WP 235 **On-line Separation and Quantification of Hyaluronan-Based Oligosaccharides Arising from Acid Hydrolysis**; Martina Hermannova<sup>1</sup>; Dagmar Cozikova<sup>1</sup>; Daniela Smejkalova<sup>1</sup>; Jaroslav Pavlik<sup>1</sup>; Karel Lemr<sup>2</sup>; Vladimir Velebny<sup>1</sup>; <sup>1</sup>Contipro Pharma, a.s., Dolni Dobrouc, Czech RepuBLIC; <sup>2</sup>Department of Analytical Chemistry – RCPTM, Olomouc, Czech Republic
- WP 236 **Quantitative Evaluation of Different Sample Preparation Protocols Identifies Optimal Protocol for LC-MS/MS Analysis of N-linked Glycans Derived from Biological Samples**; Rui Zhu; Shiyue Zhou; Yu Zhang; Parvin Mirzaei; Yehia Mechref; Texas Tech University, Lubbock, TX
- WP 237 **Release and Isolation of O-glycans: Towards a System for Studying Disorders of Protein O-glycosylation**; Kirsty Skeene<sup>1</sup>; Ed Bergström<sup>1,2</sup>; Daniel Ungar<sup>3</sup>; Graham Clarke<sup>4</sup>; Jane Thomas-Oates<sup>1,2</sup>; <sup>1</sup>Department of Chemistry, University of York, York, UK; <sup>2</sup>Centre of Excellence in Mass Spectrometry, University of York, York, UK; <sup>3</sup>Department of Biology, University of York, York, UK; <sup>4</sup>Bristol-Myers Squibb Pharmaceuticals Ltd, Moreton, UK
- WP 238 **Routine Monitoring of N-Glycans Using a Novel MS Enhancing Labeling Reagent with Quadrupole Mass Detection**; Eoin F.J. Cosgrave<sup>2</sup>; Matthew Lauber<sup>1</sup>; Stephan M. Koza<sup>1</sup>; Robert Birdsall<sup>1</sup>; Scott Berger<sup>1</sup>; Sean M. Mccarthy<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Seattle Genetics, Bothell, WA
- WP 239 **Rapid-throughput Glycomics of Human Milk for Identifying Bioactive Structures**; Jasmine Davis<sup>1</sup>; Sarah Totten<sup>2</sup>; Lauren Wu<sup>1</sup>; Evan Parker<sup>1</sup>; Carlito Lebrilla<sup>1</sup>; <sup>1</sup>UC Davis, Davis, CA; <sup>2</sup>Stanford University School of Medicine, Millbrae, CA
- WP 240 **Isolation and Characterization of Membrane Associated Glycans on Epithelial Cells upon Colonization by Pathogenic and Commensal Bacteria**; Dayoung Park; Narine Arabyan; Aline Pacheco; Bart Weimer; David Mills; Carlito Lebrilla; University of California, Davis, Davis, CA
- WP 241 **In-depth Profiling of Protein Deamidation Sites in Hen Tissue and Plasma for Integrated Glycome and Proteome Measurements**; James Mccord; Elizabeth Hecht; Becca Wysocky; James Petite; David C. Muddiman; North Carolina State University, Raleigh, NC



- WP 242 **Algorithms for Establishing Glycan Structure-Expression Relationships**; Anoop Mayampurath<sup>1</sup>; Shiyue Zhou<sup>2</sup>; Yehia Mechref<sup>2</sup>; Samuel Volchenboun<sup>1</sup>; <sup>1</sup>University of Chicago, Chicago, IL; <sup>2</sup>Texas Tech University, Lubbock, TX
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- WP 243 **Targeted Mass Spectrometric Analysis of Phosphoinositides in Complex Lipid Mixtures**; Su Hee Kim; Su Jung Kim; Hyun Ju Yoo; *Asan Institute for Life Sci, Asan Medical Center, Seoul, South Korea*
- WP 244 **Analysis of Coenzyme Qs and Their Relationship with Cardiolipin Content in Biological Samples by Shotgun lipidomics**; Miao Wang; Quan He; Chunyan Wang; Xianlin Han; *Sanford-Burnham Medical Research Institute, Orlando, FL*
- WP 245 **Quantitative Profiling of Lipid Species in Mouse Brain by Nanoflow Normal Phase Liquid Chromatography Mass Spectrometry and Data Independent Acquisition**; Reinaldo Almeida<sup>1</sup>; Christer Ejsing<sup>2</sup>; <sup>1</sup>University of Southern Denmark, Odense, Denmark; <sup>2</sup>Department of Biochemistry and Molecular Biology, Odense, Denmark
- WP 246 **Targeted Lipidomic Analysis of Eicosanoids**; Baljit Ubhi<sup>2</sup>; Jason Causon<sup>3</sup>; Fadi Abdi<sup>1</sup>; Michael Mihlan<sup>4</sup>; Romeo Ricci<sup>5</sup>; <sup>1</sup>AB SCIEX, Framingham, MA; <sup>2</sup>AB SCIEX, Redwood City, CA; <sup>3</sup>AB SCIEX, Warrington, UK; <sup>4</sup>Institut de Génétique et de Biologie Moléculaire, Strasbourg, France; <sup>5</sup>IGBMC, INSERM, CNRS, Université de Strasbourg, Strasbourg, France
- WP 247 **Quantification of the Membrane Lipidome Turnover by Metabolic <sup>15</sup>N Labeling and Ultra-High Resolution Orbitrap FTMS**; Kai Schuhmann<sup>1</sup>; Kristina Srzentic<sup>2</sup>; Konstantin O. Nagornov<sup>2</sup>; Theresa Gutmann<sup>4</sup>; Ünal Coskun<sup>4</sup>; Yury Tsybin<sup>2,3</sup>; Andrej Shevchenko<sup>1</sup>; <sup>1</sup>MPI of Molecular Cell Biology and Genetics, Dresden, Germany; <sup>2</sup>Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; <sup>3</sup>Spectroswiss Sàrl, Lausanne, Switzerland; <sup>4</sup>Paul Langerhans Institut, Dresden, Germany
- WP 248 **Simultaneous Tandem Mass Spectrometric Quantitation of Hexacosanoyl Lyso-phosphatidylcholine, Amino Acids, Acylcarnitines, and Succinylacetone in Extracts of Dried-Blood Spot Punches**; Christopher A. Haynes; Victor De Jesus; *Centers for Disease Control and Prevention, Atlanta, GA*
- WP 249 **QTRAP® LC/MS/MS Workflow for Simultaneous Characterization and Quantitation of PEGylated Liposomal Drug Formulations**; Sebastian Fabritz<sup>1</sup>; Cyrus Papan<sup>1</sup>; Pol Harvengt<sup>2</sup>; <sup>1</sup>Sciex, Darmstadt, Germany; <sup>2</sup>GSK Vaccines, Rixensart, Belgium
- WP 250 **Sulfatide Depletion Leads to a Dramatic Age-dependent Reduction of Myelin Lipid Content**; Chunyan Wang; Juan Pablo Palavicini; Linyuan Chen; Xianlin Han; *Sanford Burnham Medical Research Inst., Orlando, FL*
- WP 251 **Skyline Validation of Quantitative Measurements from High-Resolution LC-IMS-MS Lipidomics Profiling Experiments**; J. Will Thompson<sup>1</sup>; Laura Dubois<sup>1</sup>; Brian Pratt<sup>2</sup>; Michael J. Maccoss<sup>3</sup>; Giuseppe Astarita<sup>4</sup>; Brendan Maclean<sup>2</sup>; Arthur Moseley<sup>5</sup>; <sup>1</sup>Duke University School of Medicine, Durham, NC; <sup>2</sup>University of Washington, Seattle, WA; <sup>3</sup>Univ of Washington, Seattle, WA; <sup>4</sup>Waters Corporation, Milford, MA; <sup>5</sup>Duke University School of Medicine, Durham, NC
- WP 252 **Fast Sensitive Simultaneous Quantitative Measurement of Total Cholesterol and Triglycerides by LC-MRM for Coupling with Pre-Analytical Fractionation of Lipoproteins**; Michael Gardner; Zsuzsanna Kuklennyik; David M. Schieltz; Bryan Parks; Jon Rees; Lisa McWilliams; Yulanda Williamson; John R. Barr; *Centers for Disease Control and Prevention, Atlanta, GA*
- WP 253 **Label-free Quantification of Isomeric Wax Esters by Direct Infusion ESI MS/MS: A Study of Human Meibomian Gland Secretions**; Jianzhong Chen<sup>1</sup>; Kari Green<sup>2</sup>; Kelly Nichols<sup>1</sup>; <sup>1</sup>University of Alabama at Birmingham, Birmingham, AL; <sup>2</sup>University of Florida, Gainesville, FL
- WP 254 **Results of a NIST Interlaboratory Comparison Exercise for Lipidomics**; John Bowden; *NIST - Hollings Marine Laboratory, Charleston, SC*
- WP 255 **Identification and Quantification of Oxysterols using Ultra Performance Convergence Chromatography Combined with Tandem Mass Spectrometry (UPC2-MS/MS)**; Kumari Ubhayasekera<sup>1</sup>; Warunika Aluthgedara<sup>1</sup>; Jonas Bergquist<sup>2</sup>; <sup>1</sup>Department of Chemistry-BMC, Uppsala University, Uppsala, Sweden; <sup>2</sup>Science for Life Laboratory, Uppsala University, Uppsala, Sweden
- LIPIDS: ID AND STRUCTURAL ANALYSIS**  
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- WP 256 **Tandem Mass Spectrometry of Glycolipids**; Nicolas Alexander; Chrys Wesdemiotis; *The University of Akron, Akron, OH*
- WP 257 **EIEIO: Electron Ionization for Excitation of Ions from Organics for Near Complete Structural Characterization in Lipidomics**; Takashi Baba; J. Larry Campbell; *Sciex, Concord, Canada*
- WP 258 **Mechanistic Revisitation of Phospholipid Fragmentation under Collision Conditions through Formation of Ion-Dipole Intermediates and Salt Bridges**; Benoit Colsch<sup>2</sup>; Francois Fenaille<sup>2</sup>; Christophe Junot<sup>2</sup>; Jean-Claude Tabet<sup>1,2</sup>; <sup>1</sup>University Paris VI (UPMC) case 45 UMR 7201 CNRS, Paris Cedex 05, France; <sup>2</sup>CEA, iBiTec-S, SPI, Gif Sur Yvette, France
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- WP 260 **Robust Mass Spectrometry-Based Characterization of the Composition of Murrah Buffalo Milk Lipids**; Sivaramaiah Nallapeta<sup>1</sup>; Ow Sawyen<sup>1</sup>; Aparna Verma<sup>2</sup>; Kiran Ambatipudi<sup>2</sup>; <sup>1</sup>Bruker Daltonics India, Centre of Excellence, Bangalore, IN; <sup>2</sup>Indian Institute of Technology Roorkee, Roorkee, India
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- WP 263 **Rapid Phospholipid Characterization Using a Novel Intelligent Workflow on a Tribrid Orbitrap Mass Spectrometer**; Reiko Kiyonami<sup>1</sup>; David A. Peake<sup>1</sup>; Yasuto Yokoi<sup>2</sup>; Yingying Huang<sup>1</sup>; <sup>1</sup>ThermoFisher Scientific, San Jose, CA; <sup>2</sup>MKI, Tokyo, Japan
- WP 264 **Utilization of Photochemical Reactions and Tandem Mass Spectrometry to Analyze Neutral Lipids**; Hilary Brown; Lei Tan; Dr. Yu Xia; *Purdue University, Lafayette, IN*
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WP 267 **Characterization and Collision Cross Section Determination of Obesity Related Lipids Within Mouse Models Using Travelling Wave IMS-QToF Mass Spectrometry;** Gertjan Kramer<sup>1</sup>; Nicholas Dekker<sup>1</sup>; Lee A Gethings<sup>2</sup>; John P. Shockcor<sup>2</sup>; James I. Langridge<sup>2</sup>; Johannes P.C. Vissers<sup>2</sup>; Johannes M.F.G. Aerts<sup>1</sup>; <sup>1</sup>*Academic Medical Centre, University of Amsterdam, Amsterdam, Netherlands*; <sup>2</sup>*Waters Corporation, Manchester, UK*

WP 268 **A Cartesian Product Approach To Lipid A Structure Identification;** Lisa Leung; Tao Liang; Michael Wilson; Sung Hwan Yoon; Robert Ernst; David Goodlett; *University of Maryland, Baltimore, MD*

WP 269 **Specific Dissociations of Protonated N-acyl Amino Acid Mono Ethyl Esters under Resonant and Non-Resonant Excitation Conditions in FT/MS;** Toufik Toaalibi Boukerche<sup>1</sup>; Sandra Alves<sup>2</sup>; Mohamed Bouchekara<sup>3</sup>; Mohammed Belbachir<sup>4</sup>; Jean-Claude Tabet<sup>2</sup>; <sup>1</sup>*Université d'Oran BP 1524, Oran, Algeria*; <sup>2</sup>*University Paris VI (UPMC) case 45 UMR 8232 CNRS, Paris Cedex 05, France*; <sup>3</sup>*LCOMM Université de Mascara, BP 763, Mascara, Algeria*; <sup>4</sup>*Université d'Oran ES-SENIA, Oran, Algeria*

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WP 271 **New Insights into Ionisation and Fragmentation of Phospholipids through Untargeted Metabolomics with LC-ESI-Q-TOF;** Joanna Godzien<sup>2</sup>; Michal Ciborowski<sup>1</sup>; M. Paz Martinez-Alcazar<sup>2</sup>; Paulina Samczuk<sup>1</sup>; Adam Kretowski<sup>1</sup>; Coral Barbas<sup>2</sup>; <sup>1</sup>*Medical University of Bialystok, Bialystok, Poland*; <sup>2</sup>*CEMBIO, San Pablo CEU University, Madrid, Spain*

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WP 274 **Proteomics Analysis of the Cerebral Cortex after Fear Conditioning and Acute Blast Indicate Altered Metabolism and Convergence Upon Neurodegenerative Pathways;** Angela Boutte<sup>1</sup>; Joy Guingab-Cagmat<sup>2</sup>; Ahmed Moghie<sup>3</sup>; Joseph A. Caruso<sup>4</sup>; Shonnette F. Grant<sup>1</sup>; Eric Maudlin-Jeronimo<sup>5</sup>; Lawrence P. Simmons<sup>1</sup>; John Anagli<sup>2</sup>; Paul M. Stemmer<sup>4</sup>; Kevin K.W. Wang<sup>3</sup>; Frank C. Tortella<sup>1</sup>; Stephen T. Ahlers<sup>5</sup>; Raymond F. Genovese<sup>1</sup>; Jitendra R. Dave<sup>1</sup>; <sup>1</sup>*Walter Reed Army Inst. for Research, Silver Spring, MD*; <sup>2</sup>*Banyan Biomarkers, Inc., Alachua, FL*; <sup>3</sup>*University of Florida, Gainesville, FL*; <sup>4</sup>*Wayne State University, Detroit, MI*; <sup>5</sup>*Naval Medical Research Center, Silver Spring, MD*

WP 275 **Using Mass Spectrometry-based Proteomics to Study the Intracellular Mechanisms of Ion Transport in *Rhodnius prolixus* Species;** Noman Hassan; Juan Ianowski; George Katselis; *College of Medicine, University of Saskatchewan, Saskatoon, Canada*

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WP 277 **Investigation of the *in-vitro* Toxicoproteomic Response of Pulmonary Epithelial Cells to Well-Characterized Atomic Layer Deposition-Coated Carbon Nanotube Exposure;** Gina Hilton; Alexia Taylor; Christina McClure; Gregory Parsons; James Bonner; Michael Bereman; *North Carolina State University, Raleigh, NC*

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WP 279 **Label-free Shotgun Proteomics Reveal Pathways Pivotal in Pre-Neoplastic Prostate Development;** Owen E. Branson; Michael E. Hoover; Jennifer M. Thomas-Ahner; Steven K. Clinton; Michael A. Freitas; *Ohio State University, Columbus, OH*

WP 280 **High-definition Qualitative and Quantitative Proteomics of a Parkinson's Disease Zebrafish Model;** Joanne B. Connolly<sup>1</sup>; Kari E. Fladmark<sup>2</sup>; Edward Burton<sup>3</sup>; Ann Kristin Frøyset<sup>2</sup>; <sup>1</sup>*Waters, Manchester, UK*; <sup>2</sup>*University of Bergen, Bergen, Norway*; <sup>3</sup>*University of Pittsburgh, Pittsburgh, PA*

WP 281 **Development of a Targeted Proteomics Approach for the Validation of Dechlorination Biomarker Proteins from Organohalide-Respiring Bacterial (OHRB) Strains;** Manuel I. Villalobos-Solis<sup>1,2</sup>; Karuna Chourey<sup>1</sup>; Robert Hettich<sup>1</sup>; <sup>1</sup>*Oak Ridge National Laboratory, Oak Ridge, TN*; <sup>2</sup>*University of Tennessee, Knoxville, TN*

WP 282 **Proteomic Investigation of Developmental TCCD Toxicity using an Embryonic Zebrafish Model and LC MS/MS;** Michael Bereman; Antonio Planchart; Carolyn Mattingly; *North Carolina State University, Raleigh, NC*

WP 283 **Proteomic Analysis of Potential Biomarkers for Bladder Cancer in Urine Using OFFGEL Technology and Mass Spectrometry;** Emanuel Carrilho<sup>2</sup>; Juliana Alberice<sup>1</sup>; <sup>1</sup>*Institute of Chemistry of São Carlos, São Carlos, São Paulo*; <sup>2</sup>*USP, São Carlos, Brasil*

WP 284 **Comparative Analysis of Proteomes between Fragile X Mental Retardation 1 (FMR1) Knock-Out and Wild-Type Mouse Astrocytes;** Chenxi Yang; Weixiang Guo; Yue Li; Xinyu Zhao; Lingjun Li; *University of Wisconsin-Madison, Madison, WI*

WP 285 **Candidate Biomarkers for Colorectal Cancer Identified by Immune-Laser Capture Microdissection and LC-MS/MS;** Xinhua Liu; Rui Yang; Jianhui Zhu; Smathorn Thakolwiboon; David M. Lubman; *University of Michigan Medical Center, Ann Arbor, MI*

WP 286 **Mass Spectrometric Investigation of Phosphorylation of Salivary Proteins in Respect to the Cold Pressor Test;** Rachel Marvin; Brooke Saepoo; Jonathan Tomko; Kenneth Hensley; David Giovannucci; Dragan Isailovic; *University of Toledo, Toledo, Ohio*

WP 287 **Metabonomics Study of the Effects of Traditional Chinese Medicine Formula Ermiao Wan on Hyperuricemic Rats;** Zhiqiang Liu; Chen Xu; *Changchun Institute of Applied Chemistry, Changchun, China*

WP 288 **Hydroxyproline Levels in Mouse Tissue - Use of Traditional Colorimetric Assay Kit vs. High-Resolution LC/MS;** Joelle M. Onorato; Sumanta Mukherjee; John Menke; Petia Shipkova; Ashok Dongre; Arathi Krishnakumar; Ji Gao; Anthony V. Azzara; *Bristol-Myers Squibb, Princeton, NJ*

WP 289 **A Comprehensive Approach to Ranking Biomarker Candidates;** Xianyin Lai; *Indiana University School Of Medicine, Indianapolis, IN*

WP 290 **Different TMT Discovery Workflows with a Common Data Matrix Enable Pharmacodynamic Biomarker Discovery;** Ian Pike<sup>1</sup>; Claire Russell<sup>1</sup>; Vikram Mitra<sup>1</sup>; Mikko Hiltunen<sup>2</sup>; Henrik Zetterberg<sup>3</sup>; Amanda Heslegrave<sup>4</sup>; Jennifer



Pocock<sup>4</sup>; Malcolm Ward<sup>1</sup>; <sup>1</sup>Proteome Sciences, Cobham, UK; <sup>2</sup>University of Eastern Finland, Kuopio, Finland; <sup>3</sup>The Sahlgrenska Academy, University of Gothenburg, Gothenburg, Sweden; <sup>4</sup>UCL Institute of Neurology, London, UK

- WP 291 **Marker Discovery for Major Types of Animal Fibers through a Quantitative Proteomic Strategy**; Shanshan Li; Qichen Cao; Yong Zhang; Zhidan Zhang; Yun Xiong; Wenqing Shui; *Tianjin Institute of Industrial Biotechnology, CAS, Tianjin, China*
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- WP 294 **Proteomic Discovery and Validation of Biomarkers distinguishing Benign from Malignant Lung Nodules**; Simona G. Codreanu; Pierre P. Massion; Daniel C. Liebler; *Vanderbilt University School of Medicine, Nashville, TN*
- WP 295 **Study of Protein Breakdown following Traumatic Brain Injury by Mass Spectrometry-Based Proteomics**; Manasi Mangonkar<sup>1</sup>; David Powell<sup>1</sup>; Richard A. Yost<sup>1</sup>; Kari Green<sup>1</sup>; Kevin Wang<sup>1,2</sup>; <sup>1</sup>University of Florida, Gainesville, FL; <sup>2</sup>Department of Psychiatry & Neuroscience, Gainesville, FL
- WP 296 **Development and Application of a Simple Nano-Proteomic Platform (SNaPP) for Effective Analysis of Sub-microgram Proteomic Samples**; Paul D. Piehowski<sup>1</sup>; Eric L. Huang<sup>1</sup>; Daniel J. Orton<sup>1</sup>; Moore J. Ronald<sup>1</sup>; William B. Chrisler<sup>1</sup>; Rosalie K. Chu<sup>1</sup>; Kristin E. Burnum-Johnson<sup>1</sup>; Xiaofei Sun<sup>2</sup>; Sudhansu K. Dey<sup>2</sup>; Liu Tao<sup>1</sup>; Wei-Jun Qian<sup>1</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>Pacific Northwest National Lab, Richland, WA; <sup>2</sup>Cincinnati Children's Hospital Medical Center, Cincinnati, OH

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- WP 301 **Absolute Quantification of Apolipoprotein A1 using**

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- WP 302 **Pharmacodynamic Biomarkers to Monitor Dystrophin Replacement Therapies in Duchenne Muscular Dystrophy**; Haeri Seol; Meng H Han; Kristy J. Brown; Aiping Zhang; Margaret E Benny Klimek; Maria Candida Vila; Kanneboyina Nagaraju; Eric P Hoffman; Yetrih Hathout; *Children's National Medical Center, Washington, DC*
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- WP 305 **Novel iDiLeu Labeling Coupled with High-Resolution Mass Spectrometry for Absolute Quantification of Candidate Biomarkers in Preclinical Alzheimer's Disease**; Xiaofang Zhong; Qing Yu; Jingxin Wang; Tyler Greer; Ozioma Okonko; Lingjun Li; *University of Wisconsin-Madison, Madison, WI*
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- WP 310 **Deconvolution of MS/MS from Mixed Chemical Species**; David Cox; Gordana Ivosev; Lyle Burton; J.C. Yves Leblanc; *SCIEX, Toronto, ON, Canada*
- WP 311 **DIA-Umpire: Comprehensive Computational Framework for Data Independent Acquisition Proteomics**; Chih-Chiang Tsou<sup>1</sup>; Dmitry Avtonomov<sup>1</sup>; Brett Larsen<sup>2</sup>; Monika Tucholska<sup>2</sup>; Hyungwon Choi<sup>3</sup>; Anne-Claude Gingras<sup>2</sup>; Alexey Nesvizhskii<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>Lunenfeld-Tanenbaum Research Institute, Toronto, Canada; <sup>3</sup>National University of Singapore, Singapore, Singapore
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- Fujimoto; Christopher C Overall; Michael G Degan; Bryson C Gibbons; Samuel O Purvine; Mary S Lipton; Richard D Smith; *Pacific Northwest National Lab, Richland, WA*
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- WP 314 **Improving DIA Peptide Identification via Local Time Profile Similarity**; [Heydar Maboudi Afkham](#)<sup>1</sup>; Sangtae Kim<sup>2</sup>; Lukas Käll<sup>1</sup>; <sup>1</sup>Royal Institute of Technology - KTH, Stockholm, Sweden; <sup>2</sup>Pacific Northwest National Laboratory - PNNL, Richland, WA
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- WP 320 **High Scoring Decoys in Database Search**; [Andy Kong](#); Alexey Nesvizhskii; *University of Michigan, Ann Arbor, MI*
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- WP 327 **DeMixQ: Novel Peptide Propagation Scheme for Label-Free Quantification Solves the Problem of Missing Values in Data-Dependent Acquisition**; [Bo Zhang](#)<sup>1</sup>; Lukas Käll<sup>2</sup>; Roman Zubarev<sup>1</sup>; <sup>1</sup>Karolinska Institutet, Stockholm, Sweden; <sup>2</sup>Royal Institute of Technology, Stockholm, Sweden
- WP 328 **Chimeric MS/MS Spectra Identification using MS Amanda**; [Viktoria Dorfer](#)<sup>1</sup>; Sergey Maltsev<sup>2</sup>; Stephan Winkler<sup>1</sup>; Karl Mechtler<sup>2, 3</sup>; <sup>1</sup>University of Applied Sciences Upper Austria, Hagenberg, Austria; <sup>2</sup>Research Institute of Molecular Pathology (IMP), Vienna, Austria; <sup>3</sup>Institute of Molecular Biotechnology (IMBA), Vienna, Austria
- WP 329 **Supervised, Image-Based Analysis of Triple-SILAC Labeled Phospho-Peptides**; [Peter Askovich](#)<sup>1</sup>; Frank Schmitz<sup>1, 2</sup>; Alan Diercks<sup>1</sup>; Alan Aderem<sup>1</sup>; <sup>1</sup>Seattle Biomedical Research Institute, Seattle, WA; <sup>2</sup>Celgene, Seattle, WA
- WP 330 **Counting and Label-Free Approaches to Identify PTM Biomarkers of Cardiovascular Disease in a Mouse Model**; [Jean L. Spencer](#); Christian F. Heckendorf; Deborah A. Siwik; Wilson Colucci; Richard A. Cohen; Catherine E. Costello; Mark E. McComb; *Boston University School of Medicine, Boston, MA*
- WP 331 **Detection of Toxicity of Bioactivated Compounds using Diagnostic Fragment Detection Software with MS2 Data**; [Bruce D. Pascal](#); Xiaohai Li; Anthony Carvalloza; Michael D. Cameron; *The Scripps Research Institute, Scripps Florida, Jupiter, FL*
- WP 332 **An Integrated Workflow for Peptide Identification Based on the High Resolution Mass Spectrometry Data**; [Hao Chi](#); Wen-Feng Zeng; Long Wu; Kun He; Chao Liu; Rui-Xiang Sun; Si-Min He; *Institute of Computing Technology, CAS, China*
- WP 333 **proteoQC: An R/Bioconductor Package for Quality Assessment of MS-based Proteomics Data**; [Bo Wen](#)<sup>1</sup>; Laurent Gatto<sup>2</sup>; Shaohang Xu<sup>1</sup>; Ruo Zhou<sup>1</sup>; Zhe Ren<sup>1</sup>; Baojin Zhou<sup>1</sup>; Zhilong Lin<sup>1</sup>; Quanhui Wang<sup>1, 3</sup>; Jin Zi<sup>1</sup>; Shida Zhu<sup>1</sup>; Yong Hou<sup>1</sup>; Liang Lin<sup>1</sup>; Xun Xu<sup>1</sup>; Siqi Liu<sup>1</sup>; <sup>1</sup>BGI-Shenzhen, Shenzhen, China; <sup>2</sup>University of Cambridge, Cambridge, UK; <sup>3</sup>Beijing Institute of Genomics, Beijing, China
- WP 334 **DPR, a Novel Measure to Evaluate the Quantitation Accuracy of Different Software Tools in Quantitative Proteomics**; [Chao Liu](#); Zuo-Fei Yuan; Yan Fu; Hao Chi; Wen-Feng Zeng; Rui-Xiang Sun; Si-Min He; *ICT, CAS, Beijing, China*
- WP 335 **An Improved Random Decoy Database Construction Strategy for Estimating False Positives and False Discovery Rates in Shotgun Proteomics**; [Guanghui Wang](#); Marjan Gucek; *Proteomics Core, NHLBI, NIH, Bethesda, MD*
- WP 336 **Peptide Informatics: Carrying Peptide Level Quantitation through the Bioinformatic Workflow Enables New Enrichment Methodology**; [Michael Smallegan](#)<sup>1</sup>; James Dowell<sup>1, 2</sup>; <sup>1</sup>Wisconsin Institute for Discovery, Madison, WI; <sup>2</sup>UW-Madison, Madison, WI
- WP 337 **Towards Modified Peptide Identification using Blazmass**; [Lin He](#); Robin Park; John Yates; *The Scripps Research Institute, La Jolla, CA*
- WP 338 **An Intensity Based Quantification Strategy for HR-PRM**





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- WP 339 **Impact of Various Gel Storage Conditions on Overall LC-MS Identification Outcome;** Michaela Scigelova<sup>1</sup>; Petra Dvorakova<sup>2</sup>; Lenka Hernychova<sup>2</sup>; Martina Zahradnikova<sup>2</sup>; Torsten Ueckert<sup>1</sup>; Bernard Delanghe<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, Bremen, Germany*; <sup>2</sup>*Masarykuv onkologicky ustav, Brno, Czech Republic*
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- WP 340 **Analysis of Angiotensinogen Redox Switch Involved in the Pathogenesis of pre-Eclampsia by Targeted LC-MS/MS;** Lina Dahabiyeh<sup>1</sup>; David Tooth<sup>2</sup>; Rob Layfield<sup>2</sup>; Aiwu Zhou<sup>3</sup>; Robin Carrell<sup>4</sup>; Yahui Yan<sup>4</sup>; Randy Read<sup>4</sup>; David Barrett<sup>1</sup>; <sup>1</sup>*University of Nottingham, School of Pharmacy, Nottingham, UK*; <sup>2</sup>*Biomedical Sciences School, Nottingham University, Nottingham, UK*; <sup>3</sup>*Shanghai Jiatong University, Shanghai, China*; <sup>4</sup>*University of Cambridge, Cambridge, UK*
- WP 341 **Optimization of Signature Peptide Formation for LC-MS/MS Quantification of Humanized Monoclonal Antibody Trastuzumab in Human Serum;** Luc Bouchard; Marie-Claude Théberge; Nadine Boudreau; Ann Lévesque; *inVentiv Health Clinical, Québec, Canada*
- WP 342 **Quantification of Low Abundant Amino Acid Misincorporations by Multidimensional Chromatographic Enrichment and Selected Reaction Monitoring (SRM);** Raffaella Garofalo<sup>1</sup>; Ingo Wohlgemuth<sup>1</sup>; Christof Lenz<sup>1,2</sup>; Henning Urlaub<sup>1,2</sup>; Marina V. Rodnina<sup>1</sup>; <sup>1</sup>*Max Planck Institute for Biophysical Chemistry, Goettingen, Germany*; <sup>2</sup>*University Medical Center (UMG), Goettingen, Germany*
- WP 343 **A Single, Rapid Integrated Method to Quantify the Anti-Inflammatory Protein, TSG-6, by On-Column Proteolytic Digestion Followed by LC/ESI-MSMS;** Joshua Emory<sup>2</sup>; Benjamin Oyler<sup>1</sup>; Timothy Varney<sup>2</sup>; Kathleen Housman<sup>2</sup>; Jonathan Oyler<sup>2</sup>; <sup>1</sup>*University of Maryland, Baltimore, Whiteford, MD*; <sup>2</sup>*USA Medical Research Institute of Chemical Defense, Aberdeen Proving Ground, MD*
- WP 344 **Systematic Comparison of Internal Standard Platforms for Absolute Protein Quantification of Cytokines by MRM-MS;** Kerry Bauer<sup>1,2</sup>; Illarion Turko<sup>1,2</sup>; Karen Phinney<sup>1</sup>; <sup>1</sup>*National Institute of Standards and Technology, Gaithersburg, MD*; <sup>2</sup>*Institute for Bioscience and Biotechnology Researc, Rockville, MD*
- WP 345 **Absolute Quantification of Key Pathway Proteins Reveals SOS1 as the Bottleneck of ERK Response in the Ras-MAPK Pathway;** Tujin Shi<sup>1</sup>; Mario Niepel<sup>2</sup>; Carrie D. Nicora<sup>1</sup>; Yuqian Gao<sup>1</sup>; Thomas L. Fillmore<sup>3</sup>; William B. Chrisler<sup>1</sup>; Matthew J. Gaffrey<sup>1</sup>; Ronald J. Moore<sup>1</sup>; Tao Liu<sup>1</sup>; David G. Camp II<sup>1</sup>; Richard D. Smith<sup>1</sup>; Karin D. Rodland<sup>1</sup>; Peter K. Sorger<sup>2</sup>; H. Steven Wiley<sup>3</sup>; Wei-Jun Qian<sup>1</sup>; <sup>1</sup>*PNNL, Richland, WA*; <sup>2</sup>*Harvard Medical School, Boston, MA*; <sup>3</sup>*EMSL, PNNL, Richland, WA*
- WP 346 **Gaining Insight into Complex Biology During the Drug Discovery Process Using Quantitative Immunocapture MicroFlow LC-MS/MS;** Eugene F. Ciccimaro; Bogdan Slecza; Yongxin Zhu; John T. Mehl; Bryan Parks; Susan Kuklennyik; David M. Schieltz; Michael Gardner; Jon Rees; McWilliams Lisa; Yulanda Williamson; John R. Barr; *Centers for Disease Control and Prevention, Atlanta, GA*
- WP 358 **Multiplexed Mass Spectrometry Analysis of Metabolic Reprogramming in Colorectal Cancer Cells;** Josiah Hutton<sup>1</sup>; Lisa Zimmerman<sup>1,2</sup>; Robbert Slebos<sup>1,2</sup>; Daniel Liebler<sup>1,2</sup>; <sup>1</sup>*Vanderbilt University Medical Center, Nashville, TN*; <sup>2</sup>*Jim Ayers Institute, Nashville, TN*
- WP 359 **Evaluating Challenges Associated with Fast Quantitation of Multiple Proteins using a UHPLC-triple Quadrupole Electrospray Ionization Mass Spectrometer (LC-QQq ESI-MS);** Rohana Liyanage<sup>1</sup>; Jennifer Gidden<sup>1</sup>; Jeremy Post<sup>2</sup>; David Colquhoun<sup>2</sup>; Ben Figard<sup>3</sup>; Jackson O. Lay Jr<sup>1</sup>; <sup>1</sup>*University of Arkansas, Fayetteville, AR*; <sup>2</sup>*Shimadzu Scientific Instruments, Columbia, MD*; <sup>3</sup>*Shimadzu Scientific, Houston, TX*
- WP 360 **A Complete Solution for the Reproducible and Standardized Evaluation of Candidate CVD Protein Biomarkers in Human Plasma;** Andrew Percy<sup>1</sup>; Juncong Yang<sup>1</sup>; Darryl Hardie<sup>1</sup>; Nicole Sessler<sup>1</sup>; Yassene Mohammed<sup>1,2</sup>; Christoph Borchers<sup>1,3</sup>; <sup>1</sup>*University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada*; <sup>2</sup>*Center for Proteomics & Metabolom., Leiden UMedCtr, Leiden, The Netherlands*; <sup>3</sup>*Dept. of Biochem. & Microbiol., Univ. of Victoria, Victoria, BC, Canada*
- WP 361 **Toward the Development of Scheduled MRM Analysis for Proteome-Wide Profiling of GTP-binding Proteins;** Ming Huang; Yongsheng Xiao; Yinsheng Wang; *University of California - Riverside, Riverside, CA*
- WP 362 **Affinity Tag- and in vitro Expression-Based Synthesis of Stable Isotope-Labeled Peptides for Quantitative Proteomics;** Feng Xian<sup>1,2</sup>; Quanhui Wang<sup>1,2</sup>; Haidan Sun<sup>1</sup>; Xiaomin Lou<sup>1</sup>; Jin Zi<sup>2</sup>; Guixue Hou<sup>1,2</sup>; Lin Wu<sup>1</sup>; Siqi Liu<sup>1,2</sup>; <sup>1</sup>*Beijing Institute of Genomics, CAS, Beijing, China*; <sup>2</sup>*BGI-Shenzhen, Shenzhen, China*
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- WP 363 **Natural Flanking Sequences for Peptides Included in Quantification Concatamer Internal Standard;** Crystal Cheung<sup>1</sup>; Kyle Anderson<sup>2</sup>; Meiyao Wang<sup>1</sup>; Illarion Turko<sup>2</sup>; <sup>1</sup>*IBBR, Rockville, Maryland*; <sup>2</sup>*NIST, Gaithersburg, MD*
- WP 364 **Quantification of Histone Post-Translational Modifications by Mass Spectrometry;** Zuo-Fei Yuan<sup>1</sup>; Shu Lin<sup>1</sup>; Rosalynn C. Molden<sup>2</sup>; Xing-Jun Cao<sup>1</sup>; Natarajan V. Bhanu<sup>1</sup>; Xiaoshi Wang<sup>1</sup>; Simone Sidoli<sup>1</sup>; Shichong Liu<sup>1</sup>; Benjamin A. Garcia<sup>1</sup>; <sup>1</sup>*University of Pennsylvania, Philadelphia, PA*; <sup>2</sup>*Princeton University, Princeton, NJ*
- WP 365 **Ultrafast and Robust Optimization of Peptide MRMs Using a Fast-Scanning Triple Quadrupole Mass Spectrometer;** Jeff Dahl; David Colquhoun; *Shimadzu Scientific Instruments, Columbia, MD*
- WP 366 **Generation of Reproducible Mass Spectra by MALDI and Its Application to Quantification of Peptides and Proteins;** Sung Hee Ahn<sup>1</sup>; Jeong Hee Moon<sup>2</sup>; Seong Hoon Lee<sup>1</sup>; Myung Soo Kim<sup>1</sup>; <sup>1</sup>*Seoul National University, Seoul, Korea*; <sup>2</sup>*Medical Proteomics Research Center, KRIBB, Daejeon, Korea*
- WP 367 **Bioanalysis of Therapeutic Peptides by LC/MS/MS: Challenges and Strategies;** Eric Ma; Moucun Yuan; William Mylott; Bruce Hidy; Rand Jenkins; *PPD, Richmond, VA*
- WP 368 **On-line Preservation for in vivo Microdialysis with MS<sup>3</sup> Quantification and Dynamic Monitoring of Endogenous Opioids in the Anterior Cingulate Cortex;** Nicholas Laude<sup>1</sup>; Diana Meske<sup>1</sup>; Kramer Catherine<sup>1</sup>; Eric Lemister<sup>1</sup>; Edita Navratilova<sup>1</sup>; Frank Porreca<sup>1,2</sup>; <sup>1</sup>*The University of Arizona, Tucson, AZ*; <sup>2</sup>*Mayo Clinic, Phoenix, AZ*
- WP 369 **Efficient Micro-Scale Basic Reverse Phase Peptide Fractionation for Global and Targeted Proteomics;** Hyoung Joo Lee; Hye-Jung Kim; Daniel C. Liebler; *Department of Biochemistry, Vanderbilt University, Nashville, TN*
- WP 370 **Application of a Fluorescent Peptide Assay to the Optimization of Peptide Generation from Patient-derived Breast Cancer Xenografts;** Yiling Mi<sup>1</sup>; Petra Erdmann-Gilmore<sup>1</sup>; Rose Connors<sup>1</sup>; Matthew R. Meyer<sup>1</sup>; Shunqiang Li<sup>1</sup>; Sherri R. Davies<sup>1</sup>; Matthew J. Ellis<sup>2</sup>; R. Reid Townsend<sup>1</sup>; <sup>1</sup>*Washington University School of Medicine, St.*

- WP 371 *Louis, MO; <sup>2</sup>Baylor College of Medicine, Houston, TX*  
**Identification and Characterization of Impurities in a VLP-Peptide Conjugate Vaccine by LC-MS; Melissa Thompson**; Barbara Kelly; Kevin Bullock; John Amery; *Pfizer Inc., Chesterfield, MO*
- WP 372 **Absolute Quantification of Flavin-containing Monooxygenases (FMOs) in Human Liver Microsomes by UPLC-MS/MS-based Targeted Quantitative Proteomic Approach; Yao Chen**; Michael Zhuo Wang; *Pharmaceutical Chemistry, University of Kansas, Lawrence, KS*
- WP 373 **Higher Isobaric Multiplexing for Discovery Proteomics of Genomically-Characterized Patient-Derived Breast Cancer Xenografts; Xuya Wang**<sup>3</sup>; Petra Erdmann-Gilmore<sup>1</sup>; Alan E. Davis<sup>1</sup>; Henry W. Rohrs<sup>1</sup>; Shunqiang Li<sup>1</sup>; Sherri R. Davies<sup>1</sup>; Matthew J. Ellis<sup>1</sup>; Ryan Bomgarden<sup>4</sup>; Rosa Viner<sup>2</sup>; John C. Rogers<sup>4</sup>; David Fenyó<sup>3</sup>; Jason M. Held<sup>1</sup>; R. Reid Townsend<sup>1</sup>; <sup>1</sup>Washington University, St Louis, MO; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA; <sup>3</sup>New York University, New York, NY; <sup>4</sup>Thermo Fisher Scientific, Rockford, IL
- WP 374 **Using Mass Spectrometry in Protein Quantification for Influenza Vaccine Quality Control: To Label or Not to Label? Terry D. Cyr**; Daryl G.S. Smith; Lisa Walrond; Marybeth Creskey; Genevieve Gingras; Yves Aubin; *Health Canada, Ottawa, Canada*
- WP 375 **Fast, Sensitive, Robust SPE-LC-MS/MS Method for Quantitation of Insulin Analogues in Clinical Studies; Lei Xiong**<sup>1</sup>; Witold Woroniecki<sup>1</sup>; Rahul Baghla<sup>2</sup>; Suma Ramagiri<sup>3</sup>; Gary Impey<sup>3</sup>; Hua-Fen Liu<sup>1</sup>; <sup>1</sup>AB SCIEX, Redwood City, California; <sup>2</sup>AB SCIEX, Gurgaon, India; <sup>3</sup>AB SCIEX, Concord, ON
- WP 376 **LC/MS/MS Analysis of Oxytocin and ARG-Vasopressin in Human Plasma/Serum using Strata™-X-CW Solid Phase Extraction and a Luna PFP(2) HPLC Column; Xianrong (Jenny) Wei**; Sean Orłowicz; *Phenomenex, Torrance, CA*
- WP 377 **Development of the Ultra-Sensitive Liquid Chromatography-Tandem Mass Spectrometry Method for Insulin Lispro; Xiaodong Zhu**; Thomas Lloyd; Jingguo Hou; Jerry Gardella; Edward Wells; Steve Unger; *Worldwide Clinical Trials Drug Development Solutio, Austin, TX*
- WP 378 **LC-MS/MS Quantification of SOM230 (Pasireotide), a Cyclic Peptide, in Monkey Plasma; Yunlin Fu**; Wenkui Li; Jimmy Flarakos; Francis Tse; *Novartis Institutes for Biomedical Research, East Hanover, NJ*
- WP 379 **High Throughput Quantitation of 46 Histone PTMs through Unscheduled SRM-based Method Development on a Nano-HPLC Triple Quadrupole Platform; Jenny Chen**<sup>1</sup>; Tommy Cheung<sup>2</sup>; David Arnott<sup>2</sup>; Yan Chen<sup>1</sup>; Keith Waddell<sup>1</sup>; Cindy Lai<sup>1</sup>; <sup>1</sup>ThermoFisher Scientific Inc., San Jose, CA; <sup>2</sup>Genentech, South San Francisco, CA
- WP 380 **MRM Analysis together with ATP Affinity Probes for the Quantitative Discovery of Target Kinases of MM-3-51 in Du-145 Cells; Weili Miao**; Lei Guo; Yinsheng Wang; *Riverside, CA*
- WP 381 **Impact of Mobile Phase Modifiers and Supercharging Reagents on Charge State Distribution and Sensitivity of Therapeutic Peptides by LC-HRMS; Jean-Nicholas Mess; Daniel Villeneuve**; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*
- WP 382 **Development of an LC-MS/MS Method for Variegin Quantitation: Application to Pre-Clinical Pharmacokinetic Studies; Norrapat Shih**<sup>1,2</sup>; R. Manjunatha Kini<sup>1,2</sup>; <sup>1</sup>Dept. of Biological Sciences, National University of Singapore, Singapore; <sup>2</sup>NUS Graduate School for Integrative Sciences, & Engineering, Singapore
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- WP 384 **Concomitant Analysis of Phosphoproteome and N-linked Sialoproteome by Stepwise Metal Oxide Chromatography; Miao-Hsia Lin**; Chia-Feng Tsai; Wei-Ting Lai; Pei-Yi Lin; Yu-Ju Chen; *Academia Sinica, Taipei, Taiwan*
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- WP 386 **Development and Application of a Modified Biotin Switch Assay to Quantify Sulfenic Acid Modification of Proteins; Ru Li**; Shujun Lin; Juergen Kast; *The Biomedical Research Centre, UBC, Vancouver, Canada*
- WP 387 **A Chemical Derivatization Strategy for Profiling Protein Methylation; Zhibin Ning**; Alexandra Star; Anna Mierzwa; Sylvain Lanouette; Janice Mayne; Jean-Francois Couture; Daniel Figeys; *Ottawa Institute of Systems Biology, Ottawa, Canada*
- WP 388 **Characterizing Growth Phase-Dependent Changes in the *Bacillus subtilis* Acetyloyme and Proteome using Label-Free Quantification; Todd M. Greco**<sup>1</sup>; Valerie J. Carabetta<sup>2</sup>; David Dubnau<sup>2</sup>; Ileana M. Cristea<sup>1</sup>; <sup>1</sup>Princeton University, Princeton, NJ; <sup>2</sup>New Jersey Medical School, Rutgers University, Newark, NJ
- WP 389 **Towards Global Sulfation Analysis: Integrating Weak Anion Exchange and Ultraviolet Photodissociation Mass Spectrometry with Strategic Modulation of Peptide Basicity; Michelle Robinson**<sup>1</sup>; Jennifer Brodbelt<sup>2</sup>; <sup>1</sup>University of Texas at Austin, Austin, TX; <sup>2</sup>The University of Texas, Austin, TX
- WP 390 **In-depth Mouse Muscle Ubiquitylome Characterization using diGly Enrichment Followed by MudPIT; Punitee Garyali; Whitney Smith-Kinnaman; Peter Roach; Amber Mosley**; *Indiana University SOM, Department of Biochemistry, Indianapolis, IN*
- WP 391 **Analysis Of Alexa-594 Modified Peptides By Electrospray – Ionization Mass Spectrometry And Electron-Transfer Dissociation; Julian Whitelegge**; Joseph Capri<sup>1</sup>; Piotr Ruchala<sup>1</sup>; Marcella Gilmore<sup>2</sup>; Don Laudicina<sup>2</sup>; <sup>1</sup>University of California LA, Los Angeles, CA; <sup>2</sup>Allergan Inc., Irvine, CA
- WP 392 **Single-probe Ionization Device: Application to the Detection of Sulfated Peptides and Sugars; Rachel Wovcicefski**; Ning Pan; Zhibo Yang; *University of Oklahoma, Norman, OK*
- WP 393 **Glycopeptidomics: Characterizing Global Glycoprotein and Site Heterogeneity; Robert J. Chalkley**<sup>1</sup>; Shouling Xu<sup>1,2</sup>; Peter R. Baker<sup>1</sup>; Katalin F. Medzihradzsky<sup>1</sup>; <sup>1</sup>UCSF, San Francisco, CA; <sup>2</sup>Carnegie Institution for Science, Stanford, CA
- WP 394 **Characterization of Glycopeptides by Hot Electron Capture Dissociation; Kshitij Khatri**<sup>1</sup>; Yi Pu<sup>2</sup>; Deborah R. Leon<sup>1</sup>; Catherine E. Costello<sup>2</sup>; Joseph Zaia<sup>1</sup>; Cheng Lin<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA; <sup>2</sup>Boston University, Boston, MA
- WP 395 **Discovery and Characterization of Post-Translationally Modified Peptides with No Mass Shifts; Erik T. Jansson**; Itamar Livnat; Hua-Chia Tai; Stanislav S. Rubakhin; Jonathan V. Sweedler; *University of Illinois at Urbana-Champaign, Urbana, IL*
- WP 396 **Integrated Proteomic and Glycoproteomic Analyses of Prostate Cancer Cells; Punit Shah**; Xiangchun Wang; Weiming Yang; Shadi Toghi Eshghi; Shisheng Sun; Naser Hoti; Jered Pasay; Abigail Rubin; Hui Zhang; *Johns Hopkins*



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- WP 397 **Multi-acylation of Melittin by Iyso-phosphatidylcholines (IysoPCs) and diacylphosphatidylcholines (diacylPCs) and the Enhanced Reactivity of Melittin Towards IysoPCs;** Vian S. Ismail; John M. Sanderson; Jackie A. Mosely; *Durham University, Durham, UK*
- WP 398 **Identification of S-Glutathionylated Cysteine Residues in Murine Hepatic Proteins by nLC-CID-ETD MS/MS following Immunoaffinity Enrichment;** Susana Comte-Walters; Tiffany Ancrum; Danyelle Townsend; Lauren Ball; *Medical Univ of S Carolina, Charleston, SC*
- WP 399 **Ultra-Low Flow Capillary Electrophoresis - Mass Spectrometry for Proteome Wide PTM Identification and Quantification;** Klaus Faserl; Herbert H. Lindner; *Biocenter, Division of Clinical Biochemistry, Innsbruck, Austria*
- WP 400 **pGlyco: A Novel Pipeline for the Identification of Intact Glycopeptides;** Wen-Feng Zeng<sup>1</sup>; Mingqi Liu<sup>2</sup>; Yang Zhang<sup>2</sup>; Jianqiang Wu<sup>1</sup>; Pan Fang<sup>2</sup>; Weiqian Chao<sup>2</sup>; Chao Liu<sup>1</sup>; Hao Chi<sup>1</sup>; Ruixiang Sun<sup>1</sup>; Si-Min He<sup>1</sup>; Pengyuan Yang<sup>2</sup>; <sup>1</sup>*ICT, Chinese Academy of Sciences, Beijing, China*; <sup>2</sup>*Institutes of Biomedical Sciences, Fudan University, Shanghai, China*
- WP 401 **PARP9 Inhibits ADP-ribosylation of STAT1 by PARP14;** Iwao Yamada<sup>1,2</sup>; Hideo Yoshida<sup>1,2</sup>; Hiroshi Iwata<sup>1</sup>; Masanori Aikawa<sup>1</sup>; Sasha A. Singh<sup>1</sup>; <sup>1</sup>*Brigham and Women's Hospital, Boston, MA*; <sup>2</sup>*Kowa Company, Ltd., Tokyo, Japan*
- WP 402 **ETD Fragmentation Improves the Global Analysis of Ubiquitylated Proteins;** Tanya Porras-Yakushi; Michael J Sweredoski; Sonja Hess; *Caltech, Pasadena, CA*
- WP 403 **An Improved Strategy for Characterizing Arginine Methylation using Off-Line High-pH Reversed-Phase Fractionation and Q-Exactive HF Analysis;** Kathrine B. Sylvestersen; Sara C. Larsen; Michael L. Nielsen; *NNF Center for Protein Research, Copenhagen N, Denmark*
- WP 404 **Characterization of Polyubiquitin Chains: Linear and Branched Ubiquitin Trimers;** Amanda Lee; Yeji Kim; Emma K. Dixon; Tanuja R. Kashyap; Yan Wang; David Fushman; Catherine Fenselau; *University of Maryland, College Park, MD*
- WP 405 **Global Analysis of Arginine Methylation and *in vivo* CARM1 Substrates via IAP-MS;** Evgenia Shishkova<sup>1</sup>; Lu Wang<sup>2</sup>; Alexander H. Hebert<sup>1</sup>; Michael S. Westphal<sup>3</sup>; Wei Xu<sup>2</sup>; Joshua J. Coon<sup>1</sup>; <sup>1</sup>*Department of Biomolecular Chemistry, Madison, WI*; <sup>2</sup>*Department of Oncology, Madison, WI*; <sup>3</sup>*Univ of Wisconsin, Madison, WI*
- WP 406 **Comparison and Combination of Search Engines to Discover and Characterize PTM Signatures in Biology;** Xiaoyue Jiang<sup>1</sup>; Keith Waddell<sup>1</sup>; Michael Blank<sup>1</sup>; Kai Fritzemeier<sup>2</sup>; Bernard Delanghe<sup>2</sup>; Rosa Viner<sup>1</sup>; Andreas FR Huhmer<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*Thermo Fisher Scientific, Bremen, Germany*
- WP 407 **Data Independent Acquisition Dependent Acquisition;** Richard S. Johnson; Han-Yin Yang; Michael J. Maccoss; *University of Washington, Seattle, WA*
- WP 408 **Improved Strategy for Identification of ATM/ATR Substrates on a Q Exactive HF Platform;** Sara C. Larsen; Kathrine B. Sylvestersen; Dorte B. Bekker-Jensen; Michael L. Nielsen; *NNF Center for Protein Research, Copenhagen, Denmark*
- WP 409 **A D-Amino Acid-Containing Neuropeptide Discovery Funnel;** Itamar Livnat; Hua-Chia Tai; Erik Jansson; Stanislav Rubakhin; Jonathan Sweedler; *University of Illinois at Urbana-Champaign, Urbana, IL*
- WP 410 **Identification of Amadori Products on Proteins from Roasted Peanut Extracts using MS3 Approaches and Novel Computational Methods;** Katina L. Johnson<sup>1</sup>; Geoffrey A. Mueller<sup>1</sup>; Soheila J. Maleki<sup>2</sup>; Anna Pomes<sup>3</sup>; Jason G. Williams<sup>1</sup>; <sup>1</sup>*National Institute of Environmental Health Science, Research Triangle Park, NC*; <sup>2</sup>*US Department of Agriculture, New Orleans, LA*; <sup>3</sup>*Indoor Biotechnologies, Charlottesville, VA*
- WP 411 **Characterization of Product Related Impurities of an IgG by LC-MS/MS and Middle-Down MS/MS;** Chunyan Gu<sup>1</sup>; Deyun Wang<sup>2</sup>; Huijuan Li<sup>1</sup>; Mohammed Shameem<sup>1</sup>; Yan-Hui Liu<sup>1</sup>; <sup>1</sup>*Merck, Kenilworth, NJ*; <sup>2</sup>*Lancaster Labs, Lancaster, PA*
- WP 412 **SUMOylation Dynamics in Response to Replication Stress Reveals Novel SUMO Target Proteins and SUMO Sites Relevant for Genomic Stability;** Zhenyu Xiao<sup>1</sup>; Jer-gung Chang<sup>1</sup>; Ivo Hendriks<sup>1</sup>; Jón Sigurðsson<sup>2</sup>; Jesper Olsen<sup>2</sup>; Alfred Vertegaal<sup>1</sup>; <sup>1</sup>*Leiden University Medical Center, Leiden, Netherlands*; <sup>2</sup>*Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark*
- WP 413 **Determination of the Disulfide Linkages Present in Synthetic Ssm6a, a Novel Na 1.7 Inhibitory Peptide from Centipede Venom by Partial Reduction;** John Hui; John Robinson; Chris Spahr; Justin Murray; Stone D.-H. Shi; *Therapeutic Discovery, Amgen Inc, Thousand Oaks, CA*
- WP 414 **Deep, Quantitative Coverage of the Lysine Acetylome using Novel Anti-Acetyl-Lysine Antibodies and an Optimized Proteomic Workflow;** Tanya Svinikina<sup>1</sup>; Hongbo Gu<sup>2</sup>; Jeffrey C. Silva<sup>2</sup>; Philipp Mertins<sup>1</sup>; Jana Qiao<sup>1</sup>; Shaunt Fereshetian<sup>1</sup>; Jacob D. Jaffe<sup>1</sup>; Eric Kuhn<sup>1</sup>; Namrata D. Udeshi<sup>1</sup>; Steven A. Carr<sup>1</sup>; <sup>1</sup>*Broad Institute of MIT and Harvard, Cambridge, MA*; <sup>2</sup>*Cell Signaling Technology, Inc., Danvers, MA*
- WP 415 **Isocyanic acid Neutral Loss Ion Reduce False Positive Identification of Arginine Citrullination in Database Searches of LC-MS/MS Data;** Tatiana N. Boronina<sup>1</sup>; Raghothama Chaerkady<sup>2</sup>; Maximilian Konig<sup>1</sup>; Felipe Andrade<sup>1</sup>; Robert O'meally<sup>1</sup>; Lauren DeVine<sup>1</sup>; Robert Cole<sup>1</sup>; <sup>1</sup>*Johns Hopkins School of Medicine, Baltimore, MD*; <sup>2</sup>*Johns Hopkins University, Baltimore, MD*
- WP 416 **CESI-MS Analysis of Asparagine Deamidation and Aspartate Isomerization in Polypeptides;** Bettina Sarg; Klaus Faserl; Herbert H. Lindner; *Div. of Clin. Biochemistry, Biocenter Innsbruck, Innsbruck, Austria*
- WP 417 **Glycopeptides Automatically Assigned Using ESI-MS/MS Exact Mass Data and the MASSPEC Algorithm;** Marshall M. Siegel<sup>1</sup>; Gary Walker<sup>1</sup>; Kim Alving<sup>2</sup>; *MS Mass Spec Consultants, Fair Lawn, NJ*; <sup>2</sup>*Genzyme, Waltham, MA*
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- WP 418 **Correlation of Matrix Excited State Dynamics with Morphology and MALDI Performance;** Kris Kirmess<sup>1</sup>; Richard Knochenmuss<sup>2</sup>; Gary Blanchard<sup>3</sup>; Gary R. Kinsel<sup>1</sup>; <sup>1</sup>*Southern Illinois University Carbondale, Carbondale, Illinois*; <sup>2</sup>*Tofwerk, Seftigen, N/A*; <sup>3</sup>*Michigan State University, East Lansing, MI*
- WP 419 **Thermally Induced Dissolution of Salts in Matrix-Assisted Laser Desorption/Ionization;** Chuping Lee; I-Chung Lu; Yuan Tseh Lee; Chi-Kung Ni; *Academia Sinica, Taipei, Taiwan*
- WP 420 **The Effect of Ultra-Low Flow on the Ionization of Biotherapeutics;** Andras Guttman; *AB Sciex, San Diego, CA*
- WP 421 **Supermetallization of Peptides and Proteins during Electrospray Ionization;** Maria Indeykina<sup>1,2</sup>; Yury Kostyukevich<sup>2,4</sup>; Marina Rodchenkova<sup>1,2</sup>; Alexey Kononikhin<sup>1,2</sup>; Igor Popov<sup>2,3</sup>; Eugene Nikolaev<sup>2,4</sup>; <sup>1</sup>*Institute for Biochemical Physics, Moscow, Russian Federation*; <sup>2</sup>*Institute for Energy Problems of Chemical Physics, Moscow, Russian Federation*; <sup>3</sup>*Moscow Institute of Physics and Technology, Dolgoprudny, Russian Federation*; <sup>4</sup>*Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation*
- WP 422 **Protonation in Electrospray Ionization Mass Spectrometry;** Yixin Zou<sup>1</sup>; Georgia Dolios<sup>2</sup>; Yukui Zhang<sup>3</sup>; Rong Wang<sup>2</sup>; <sup>1</sup>*Zhejiang Haochuang Biotech Co.,Ltd,*

- Hangzhou, China; <sup>2</sup>Mount Sinai School of Med, New York, NY; <sup>3</sup>Dalian Institute Chemical Physics, CAS, Dalian, China
- WP 423 **On the Ionization Mechanism in Atmospheric Pressure Negative Ion Mass Spectrometry – The Role of Ozone and CO<sub>2</sub> –**; Valerie Derpmann<sup>1</sup>; Florian Stappert<sup>2</sup>; Hendrik Kersten<sup>2</sup>; Thorsten Benter<sup>2</sup>; <sup>1</sup>Carl Zeiss SMT GmbH, Oberkochen, Germany; <sup>2</sup>University of Wuppertal, Wuppertal, Germany
- WP 424 **Time of Ionization Spectrometry of Charged Droplets**; Carina Minardi; Arjuna Subramanian; Kaveh Jorabchi; Georgetown University, Washington, DC
- WP 425 **Fundamentals of Ionizing PEG Oligomers Using Matrix-Assisted Ionization: Determination of the Role of Cation/Anion Pairing**; Joshua Fischer; Casey Foley; Sarah Trimpin; Wayne State University, Detroit, MI
- WP 426 **Stereoselectivity of ESI-dependent Electrochemical Reactions**; Ashraf Madian<sup>1</sup>; Samantha Kaiser<sup>1</sup>; Samantha Leidner<sup>1</sup>; Denise Hayward<sup>2</sup>; Dave Loffredo<sup>2</sup>; Andrew Thiel<sup>2</sup>; Daniel Copeland<sup>1</sup>; <sup>1</sup>One2One® Pharmaceutical R&D, Hospira Inc., Lake Forest, IL; <sup>2</sup>Global Pharmaceutical R&D, Hospira Inc., Lake Forest, IL
- WP 427 **Generation and Evolution of Electronically Excited Species in Spark Discharge Plasmas - A Time and Mass Resolved Study**; Sebastian Klopotoski; Hendrik Kersten; Thorsten Benter; University of Wuppertal, Wuppertal, Germany
- WP 428 **Formate Actuated Reduction of Organic Molecules During Electrospray Ionization**; Peifeng Hu; Manorama Tummala; Baxter Healthcare, Round Lake, IL
- WP 429 **Influence of Transfer Capillary Temperature on Adduct Formation in AP-MALDI MS**; Anna Schultheis; Bernhard Spengler; Analytical Chemistry, Giessen, Germany
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- WP 430 **Laser Ablation Atmospheric Pressure Photoionization on a Portable Ion Trap Mass Spectrometer**; Yeni P. Yung; Igor V. Veryovkin; Yang Cui; Luke Hanley; University of Illinois at Chicago, Chicago, IL
- WP 431 **Metabolic Analysis of Single Human Cells by Capillary Microsampling Electrospray Ionization Mass Spectrometry and Stable Isotope Labeling**; Linwen Zhang<sup>1</sup>; Linda L. Allworth<sup>2</sup>; Akos Vertes<sup>1</sup>; <sup>1</sup>the George Washington University, Washington, DC; <sup>2</sup>Thomas Jefferson HS for Science and Technology, Alexandria, VA
- WP 432 **Single-Step Elution and Nib-Based Electrospray Ionization from Noviplex Sample Collection Cards**; Steven L. Reeber; Gary L. Glish; University of North Carolina at Chapel Hill, Chapel Hill, NC
- WP 433 **Study of Biological Samples with a Home-Built Low-Temperature-Plasma Mass Spectrometry Imaging (LTP-MSI) System**; Abigail Moreno Pedraza; Robert Winkler; CINVESTAV Unidad Irapuato, Irapuato, Mexico
- WP 434 **Comparison of Air and Nitrogen Gas Sources for DART Mass Spectrometry**; William A. Harris; Douglas B. Henderson; Johnny K. Ho; Danielle N. Dickinson; Northrop Grumman, Linthicum Heights, MD
- WP 435 **Improved Spatial Resolution for Mid-IR Laser Ablation Electrospray Ionization Mass Spectrometry in Transmission Geometry**; Richard Thurston; Rachelle Jacobson; Akos Vertes; George Washington University, Washington, District of Columbia
- WP 436 **Direct Tissue Analysis And Characterization Of Unsaturated Lipids Using a Miniature Mass Spectrometer**; Ran Zou; Yuan Su; Xiao Wang; Leelyn Chong; Yu Xia; Zheng Ouyang; Purdue University, West Lafayette, IN
- WP 437 **Co-registered Topographical, Band-Excitation Nanomechanical and Mass Spectral Imaging using a Combined Atomic Force Microscopy/Mass Spectrometry Platform**; Olga Ovchinnikova; Tamin Tai; Vera Bocharova; Mahmut Baris Okatan; Alex Belianinov; Vilmos Kertesz; Stephen Jesse; Gary J. Van Berkel; Oak Ridge National Laboratory, Oak Ridge, TN
- WP 438 **Gas Assisted AC Pipette Tip Electrospray Source**; Yunging Huang; Gong-Yu Jiang; Chao Gao; Qiao Jin; Wenjian Sun; Shimadzu Research Laboratory(Shanghai) Co.,Ltd., Shanghai, China
- WP 439 **Cross-platform Applicability of DESI-MSI – Effect of Ion Source Setups and MS Analysers on Performance and Information Recovery**; Jocelyn Tillner<sup>1</sup>; Emrys Jones<sup>1</sup>; Steve Pringle<sup>2</sup>; Tamas Karancsi<sup>3</sup>; James L Walsh<sup>4</sup>; Ian Gilmore<sup>5</sup>; Josephine Bunch<sup>5</sup>; Zoltan Takats<sup>1</sup>; <sup>1</sup>Imperial College London, London, UK; <sup>2</sup>Waters Corporation, Wilmslow, UK; <sup>3</sup>Waters Research Centre, Budapest, Hungary; <sup>4</sup>University of Liverpool, Liverpool, UK; <sup>5</sup>National Physical Laboratory, Teddington, UK
- WP 440 **On-line Planar Chromatography/Mass Spectrometry using Spray Ionization**; Michael Wei; Elizabeth Dhummakupt; Richard A. Yost; University of Florida, Gainesville, FL
- WP 441 **Mass Spectrometry on the Go**; Christopher Pulliam<sup>1</sup>; Ryan Bain<sup>1</sup>; Joshua Wiley<sup>2</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>California Institute of Technology, Pasadena, CA
- WP 442 **Comparative Study of LC-MS Analysis of Peptide Mixtures by Thermal Ionization under Ambient Conditions and ESI**; Evgeny Kukaev<sup>1,2</sup>; Alexey Kononikhin<sup>1,3</sup>; Igor Popov<sup>1,2</sup>; Eugene Nikolaev<sup>1,3</sup>; <sup>1</sup>Moscow Institute of Physics and Technology, Moscow, Russia; <sup>2</sup>Emanuel Institute of Biochemical Physics, Moscow, Russia; <sup>3</sup>Institute for Energy Problems of Chemical Physics, Moscow, Russia
- WP 443 **Study of Spray Ionization and Ion Transfer for Miniature Mass Spectrometers**; Xiao Wang; Yue Ren; Xiaoyu Zhou; Zheng Ouyang; Purdue University, West Lafayette, IN
- WP 444 **The Microwave Plasma Torch as a Combined Molecular and Atomic Ambient Ionization Source**; Kenyon Evans-Nguyen<sup>1</sup>; Ashley Windom<sup>1</sup>; Colleen Quinn<sup>1</sup>; Hilary Brown<sup>2</sup>; Spiros Manolakos<sup>3</sup>; Theresa Evans-Nguyen<sup>3</sup>; <sup>1</sup>University of Tampa, Tampa, FL; <sup>2</sup>Purdue University, West Lafayette, IN; <sup>3</sup>The Charles Stark Draper Laboratory, Inc., Tampa, FL
- WP 445 **Novel Spray-from-Tissue Ionization Method for Online and Offline Neurosurgery Assistance: Identification of Profiles by FTICR and Quadrupole Ion Trap MS**; Igor Popov<sup>1,2</sup>; Evgeny Zhvansky<sup>1,3</sup>; Denis Bormotov<sup>1,3</sup>; Vsevolod Shurkhay<sup>4</sup>; Maria Indeykina<sup>2,3</sup>; Yury Kostyukevich<sup>3,5</sup>; Alexey Kononikhin<sup>1,3</sup>; Natalia Starodubtseva<sup>1,2</sup>; Alexander Potapov<sup>4</sup>; Eugene Nikolaev<sup>3,5</sup>; <sup>1</sup>Moscow Institute of Physics and Technology, Dolgoprudny, Russian Federation; <sup>2</sup>Institute for Biochemical Physics, Moscow, Russian Federation; <sup>3</sup>Institute for Energy Problems of Chemical Physics, Moscow, Russian Federation; <sup>4</sup>Burdenko Neurosurgical Institute, Moscow, Russian Federation; <sup>5</sup>Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation
- WP 446 **Direct Coupling of Solid Phase Microextraction (SPME) to Mass Spectrometry: Applications in the Clinical Lab**; German Augusto Gomez-Rios; Barbara Bojko; Janusz Pawliszyn; University of Waterloo, Waterloo, Canada
- WP 447 **Multimodal Vacuum-assisted Laser Ablation/Transmission Plasma Ion Source for Real-time Reaction Monitoring**; Joel Keelor<sup>1</sup>; Chris Butch<sup>1</sup>; Charles Liotta<sup>1</sup>; Paul Farnsworth<sup>2</sup>; Facundo Fernandez<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA; <sup>2</sup>Brigham Young University, Provo, UT
- WP 448 **Desorption Capillary Photoionization**; Markus Haapala; Jaakko Teppo; Elisa Ollikainen; Iiro Kiiski; Anu Vaikkinen; Tiina J Kauppila; Risto Kostiaainen; University of Helsinki, Helsinki, Finland



- WP 449 **Development and Application of Hot-Gas-Assisted Desorption Atmospheric Pressure Chemical Ionization for Fast, Ambient Analysis of Milk;** [ZhiHao Wang](#)<sup>1</sup>; Jiang Wang<sup>1</sup>; Kun Liu<sup>1</sup>; Eric Handberg<sup>1</sup>; ShuiPing Yang<sup>2</sup>; Huanwen Chen<sup>1</sup>; <sup>1</sup>East China Institute of Tech., Nanchang, China; <sup>2</sup>East China Institute of Tech., Fuzhou, China
- WP 450 **Ultrasonic Acoustic Wave Nebulization-Mass Spectrometry (UltraAWN-MS) for Unconventional Explosives Characterization;** [Benjamin Oylar](#)<sup>1</sup>; Alexander MacKerell<sup>1</sup>; Kellie Hom<sup>1</sup>; Joseph Chipuk<sup>2</sup>; Richard Lareau<sup>3</sup>; Shivangi Awasthi<sup>1</sup>; Sung Hwan Yoon<sup>1</sup>; David Goodlett<sup>1</sup>; David Kilgour<sup>1</sup>; <sup>1</sup>University of Maryland, Baltimore, Baltimore, MD; <sup>2</sup>Signature Science, Alexandria, VA; <sup>3</sup>Dept. of Homeland Security, S&T Directorate, Atlantic City, NJ
- WP 451 **Membrane Electrospray Ionization for Direct Ultrasensitive Biomarker Quantitation in Biofluids Using Mass Spectrometry;** [Mei Zhang](#)<sup>1,2</sup>; Fankai Lin<sup>1</sup>; Jianguo Xu<sup>2</sup>; Wei Xu<sup>1</sup>; <sup>1</sup>Beijing Institute of Technology, Beijing, China; <sup>2</sup>Chinese Center for Disease Control and Prevention, Beijing, China
- WP 452 **Cell Phone Controlled ESI, MALDI Programmable Energy Wave Droplet Generation Technology With Applications;** Drew Sauter; [Andrew Sauter](#); Nanoliter, LLC, Henderson, NV
- WP 453 **Solvent Gradient Electrospray for Laser Ablation Electrospray Ionization Mass Spectrometry;** [Hang Li](#); Akos Vertes; George Washington University, Washington, DC
- WP 454 **Development of an Atmospheric Pressure Plasmaspray Ionization Source;** Jixing Liu; Junguo Dong; [Ping Cheng](#); Shanghai University, Shanghai, China
- WP 455 **Relay Electrospray Ionization: Triggering Electrospray using Ions and Charged Droplets for High Throughput Mass Spectrometry Analysis;** [Anyin Li](#); Adam Hollerbach; R. Graham Cooks; Purdue University, West Lafayette, IN
- WP 456 **Surface Acoustic Wave Nebulization Mass Spectrometry for Quantitative Analysis and Extraction of Analytes from Complex Matrices;** [Mridul Kanti Mandal](#); Marya Lieberman; Matthew M. Champion; David B. Go; University of Notre Dame, Notre Dame, IN
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- WP 457 **Singulus Pulpitum: Microfluidics Coupled with Mass Spectrometry for Multi-omics and Targeted Assays in Translational Research;** [Paul Rainville](#)<sup>1</sup>; James Murphy<sup>1</sup>; Giuseppe Astarita<sup>1</sup>; Ian Wilson<sup>2</sup>; James Langridge<sup>1</sup>; <sup>1</sup>Waters, Milford, MA; <sup>2</sup>Imperial College London, London, UK
- WP 458 **Increasing Sensitivity and Minimizing Sample Volume for the Quantification of Therapeutic and Endogenous Cyclic Peptides using an Integrated Microfluidic Device;** Erin E. Chambers; Mary Lame; [Markus Wanninger](#); Waters Corporation, Milford, MA
- WP 459 **Microfluidic Isoelectric Focusing Combined with MALDI- and nano-ESI-MS;** [Saara Mikkonen](#)<sup>1</sup>; Wolfgang Thormann<sup>2</sup>; Åsa Emmer<sup>1</sup>; <sup>1</sup>KTH Royal Institute of Technology, Stockholm, Sweden; <sup>2</sup>University of Bern, Bern, Switzerland
- WP 460 **Single-shot Capillary Zone Electrophoresis-Tandem Mass Spectrometry with Improved Interface for Large-Scale Shotgun Proteomics;** [Liangliang Sun](#)<sup>1</sup>; Alexander Hebert<sup>2</sup>; Xiaojing Yan<sup>1</sup>; Yimeng Zhao<sup>1</sup>; Michael S. Westphall<sup>2</sup>; Matthew Rush<sup>2</sup>; Guijie Zhu<sup>1</sup>; Matthew Champion<sup>1</sup>; Joshua J. Coon<sup>2</sup>; Norman J. Dovichi<sup>1</sup>; <sup>1</sup>University of Notre Dame, Notre Dame, U.S.; <sup>2</sup>University of Wisconsin-Madison, Madison, WI
- WP 461 **Improving NanoLC-MS Duty Cycle and Throughput: Three Channel Chip-based Column Switching using a Linear Flow Path;** [Amanda Berg](#); Helena Svobodova; Gary Valaskovic; New Objective, Inc., Woburn, MA
- WP 462 **Fast Response Microfabricated Dialysis-ESI Device Enabled by Monolithic Integration;** [Mason Chilmoneczyk](#); Ivan Tibavinsky; Peter Kottke; Andrei Fedorov; Georgia Institute of Technology, Atlanta, GA
- WP 463 **Improving the Detection of Thyroglobulin in Human Plasma by Combining SISCAPA Enrichment and Microflow LC/MS;** [Jay S. Johnson](#)<sup>1</sup>; Morteza Razavi<sup>2</sup>; Selena Larkin<sup>2</sup>; James Murphy<sup>1</sup>; Paul Rainville<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>SISCAPA Assay Technologies, Washington, DC
- WP 464 **Microfluidic Dynamic Isoelectric Focusing: A Novel Separation and Sampling Technique for MALDI Analysis;** [Srikanth Akinapalli](#); Shannon Wilson; Luke Tolley; Gary R. Kinsel; SIUC, Carbondale, IL
- WP 465 **Transferring an Analytical-Scale LC Method to an Integrated Microfluidic Device for Quantification of Human Insulin and 5 Analogs in Plasma;** [Erin E. Chambers](#); Mary Lame; Markus Wanninger; Waters Corporation, Milford, MA
- WP 466 **Mass Spectrometry for 2-D Materials: Methodology and Measurement of Free-Standing Graphene;** [Michael J. Eller](#)<sup>1</sup>; Chao-Kai Liang<sup>1</sup>; Serge Della-Negra<sup>2</sup>; Aaron B. Clubb<sup>1</sup>; Emile A. Schweikert<sup>1</sup>; <sup>1</sup>Department of Chemistry, Texas A&M University, College Station, TX; <sup>2</sup>Institut de Physique Nucléaire d'Orsay, UMR8608, Orsay, France
- WP 467 **The Routine Application of IonKey Micro-Flow LC/MS/MS to support in vivo Drug Discovery;** [Jason Barricklow](#); Yizhong Zhang; Christopher Holliman; Pfizer, New London, CT
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- WP 468 **Low SWaP-C Chemical Sensing Solution for Cometary Missions;** [Ashish Chaudhary](#)<sup>1</sup>; Tim Short<sup>1</sup>; Friso H.W. Van Amerom<sup>1</sup>; Emily Barrentine<sup>2</sup>; Yun Zheng<sup>2</sup>; William Brinckerhoff<sup>2</sup>; Daniel Glavin<sup>2</sup>; Paul Mahaffy<sup>2</sup>; <sup>1</sup>SRI International, St. Petersburg, FL; <sup>2</sup>NASA, Goddard Space Flight Center, Greenbelt, MD
- WP 469 **A Novel Quadrupole Mass Spectrometer Detection System;** [Raman Mathur](#); Michael G. Konicek; Rexford T. Heller; John Smith; Alan Schoen; Thermo Fisher Scientific, San Jose, CA
- WP 470 **Gas Flow Effects on the Operation and Efficiency of a DC Ion Carpet Interface with Particular Regard to Megadalton-Sized Ions;** [Staci Anthony](#); Benjamin Draper; Martin Jarrold; Indiana University, Bloomington, IN
- WP 471 **Comparison of Square and Round Core Fibres for MALDI MS in Lipid Standard and Tissue Imaging Studies;** [Rory T. Steven](#)<sup>1</sup>; Alan M. Race<sup>1</sup>; Elizabeth C. Randall<sup>1,2</sup>; Josephine Bunch<sup>1,3</sup>; <sup>1</sup>National Physical Laboratory, Teddington, UK; <sup>2</sup>The University of Birmingham, Birmingham, UK; <sup>3</sup>The University of Nottingham, Nottingham, UK
- WP 472 **Time-Frequency Transform Ion Trap Mass Spectrometry with Ion Collision Cross Section Measurement Capability;** [Muyi He](#); Dan Guo; Ting Jiang; Wei Xu; Beijing Institute of Technology, Beijing, China
- WP 473 **There's Plenty of Room at the Bottom: A Micro-Pixelated Position Sensitive Detector for Performance Improvement of a QMS Instrument;** [S.U.A.H. Syed](#)<sup>1,2</sup>; Gert B. Eijkel<sup>1</sup>; Simon Maher<sup>3</sup>; Fred P. M. Jjunju<sup>3</sup>; Hans R. Poolman<sup>4</sup>; Stephen Taylor<sup>3</sup>; Ron M.A. Heeren<sup>1,5</sup>; <sup>1</sup>FOM Institute AMOLF, Amsterdam, The Netherlands; <sup>2</sup>TI-COAST, Amsterdam, The Netherlands; <sup>3</sup>Department of EEE, University of Liverpool, Liverpool, UK; <sup>4</sup>Omics2Image, Amsterdam, The Netherlands; <sup>5</sup>M4I, University of Maastricht, Maastricht, The Netherlands
- WP 474 **A Novel Ion Guide with Curved Electrode Pattern Consisting of only Two Printed Circuit Boards;** [Xiaoqiang Zhang](#); Qiao Jin; Xiaoyu Meng; Chao Gao;

- Wenjian Sun; *Shimadzu Research Laboratory, Shanghai, China*
- WP 475 **Bridging the Gap between Ion Mobility Spectrometry and an Orbitrap**; Mikhail Belov<sup>1,2</sup>; William Danielson<sup>1</sup>; David Goodlett<sup>3</sup>; <sup>1</sup>*Spectrograph LLC, Kennewick, WA*; <sup>2</sup>*Thermo Fisher Scientific, Bremen, Germany*; <sup>3</sup>*University of Maryland, Baltimore, MD*
- WP 476 **Two Dimensional MS-MS on a Q-ToF Utilising a Scanning Quadrupole Mass Filter and an Ultra Fast Data Acquisition System**; Jason L Wildgoose; Keith Richardson; Martin Green; *Waters Corporation, Wilmslow, UK*
- WP 477 **Improving Ion Transmission Efficiency by Using Dynamic Acceleration Voltage in Multipole Ion guide**; Fengtao Deng; Gang Li; Lipeng Liu; Gangqiang Li; *Focused Photonics (Hangzhou), Inc, Hangzhou, China*
- WP 478 **Optimizing a Dual-Stage, Continuous-Mode, Discrete Dynode Detector for Mass Spectrometry**; Matthew Breuer; Steve Ritzau; *Photonis USA, Sturbridge, MA*
- WP 479 **Computational Evaluation of an Ion Peak Compressor Concept for Ion Mobility Spectrometry**; Sandilya V.B. Garimella; Yehia M. Ibrahim; Gordon A. Anderson; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- WP 480 **Super Wide-Dynamic-Range Ion Detector Combined a Microchannel Plate (MCP) with a Semiconductor Device**; Hiroshi Kobayashi; Motohiro Suyama; *HAMAMATSU PHOTONICS K.K., Iwata, Japan*
- WP 481 **Fast Multiplexing of Analytical Parameters for Performance Improvements in Time-of-Flight Mass Spectrometry**; Laura McGregor<sup>1</sup>; Gerhard Horner<sup>2</sup>; Pierre Schanen<sup>2</sup>; Nick Bukowski<sup>1</sup>; <sup>1</sup>*Markes International, Llantrisant, UK*; <sup>2</sup>*five technologies GmbH, Munich, Germany*
- WP 482 **A High Pressure, Three Gas Mass Spectrometer**; John Hoyes; Keith Richardson; *Waters, Manchester, UK*
- WP 483 **Development of Novel Monolithic, Resistive Glass Tube with Multi Stage capability for Use as Reflectrons, Ion Guides and Collision Cells**; Bruce Laprade; Paula Holmes; Matthew Breuer; *PHOTONIS USA, Sturbridge, MA*
- WP 484 **Of Free Ions and Clean Rods – A Study of Contamination in Ion Guides and How to Reduce It**; Felician Muntean; Stephen Zanon; Desmond Kaplan; *Bruker Daltonics, Billerica, MA*
- WP 485 **Effective Potentials Generated in SLIM Employing Planar Arrays of RF Electrodes with DC Inserts**; Aleksey V. Tolmachev; Yehia M. Ibrahim; Sandilya V. B. Garimella; Richard D. Smith; *Pacific Northwest National Lab, Richland, WA*
- WP 486 **Development and Testing of Automatic Gain Control Algorithms for EI and LDI modes in the MOMA Mass Spectrometer**; Ryan M. Danell<sup>1</sup>; Friso H.W. Van Amerom<sup>2</sup>; Veronica Pinnick<sup>3,4</sup>; Samuel Larson<sup>4</sup>; Tom Nolan<sup>4</sup>; Xiang Li<sup>3,4</sup>; Stephanie Getty<sup>4</sup>; Ricardo Arevalo<sup>4</sup>; William Brinckerhoff<sup>4</sup>; Paul Mahaffy<sup>4</sup>; <sup>1</sup>*Danell Consulting, Inc., Winterville, NC*; <sup>2</sup>*Mini-Mass Consulting, Inc, Hyattsville, MD*; <sup>3</sup>*University of Maryland, Baltimore County, Greenbelt, MD*; <sup>4</sup>*NASA GSFC, Greenbelt, MD*
- WP 487 **Enhancing Selectivity for the Analysis of Methyl Dienelone in Urine Samples by Differential Mobility Spectrometry**; Prasanth Joseph<sup>1</sup>; Sachin Dubey<sup>2</sup>; Shobha Ahi<sup>2</sup>; Neha Bhasin<sup>1</sup>; Praveen Sharma<sup>1</sup>; Manoj Pillai<sup>1</sup>; Alka Beotra<sup>2</sup>; Shila Jain<sup>2</sup>; <sup>1</sup>*SCIEX, 121, Udyog Vihar, Phase IV, Gurgaon, India*; <sup>2</sup>*National Dope Testing Laboratory, JN Stadium Complex, East Gate, New Delhi, India*
- WP 488 **Mega-Dalton Measurement with Quadrupole Ion Trap via Direct Charge Detection**; Tseng Yao-Hsin; Wan-Zo Ho; Chun-Ching Yu; Chih-Hsiang Yang; Pin-Duo Lee; Szu-Wei Chou; Hung-Liang Hsieh; Chun-Yen Cheng; *AcroMass Technologies, Inc., Taipei, Taiwan*
- WP 489 **Parallel Ion Accumulation and Analysis for 100% Duty Cycle in Trapped Ion Mobility Spectrometry**; Mark Ridgeway; Joshua Silveira; Jacob Meier; Melvin A. Park; *Bruker Daltonics, Billerica, MA*
- WP 490 **Theory and Simulation of Spiral Ion Funnel and Related Technologies for Low-Mass Transmission**; Peter Williams; *Agilent Laboratories, Santa Clara*
- WP 491 **Development of Capillary Electrophoresis Mass Spectrometry for the Metabolic Investigation of Single Embryonic Cells in *Xenopus laevis***; Sydney Morris; Rosemary Onjiko; Peter Nemes; *The George Washington University, Washington, DC*
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- WP 492 **Analytical Challenges in Developing LC-MS/MS Methods for Mancozeb and ETU in Rat Plasma**; Changyu Quang; Ernest Capraro; William Nethero; Michael Donegan; Elizabeth Groeber; *WIL Research, Ashland, OH*
- WP 493 **A High-Efficiency Cellular Extraction System for Chemical Proteomics**; Avantika Dhabaria<sup>1</sup>; Paolo Cifani<sup>1</sup>; Casie Reed<sup>1</sup>; Hanno Steen<sup>2</sup>; Alex Kentsis<sup>1</sup>; <sup>1</sup>*Memorial Sloan-Kettering Cancer Center, New York, NY*; <sup>2</sup>*Harvard Medical School/Children's Hospital Boston, Boston, MA*
- WP 494 **Proteomic Analysis of the Components of FUS Protein Aggregates with On-Membrane Tryptic Digestion**; Jing Chen; Marisa Kamelgam; Haining Zhu; *University of Kentucky, Lexington, KY*
- WP 495 **Evaluation of Streamlined SPE Processes using Novel Column based Components prior to LC-MS/MS Analysis**; Helen Lodder<sup>1</sup>; Lee Williams<sup>1</sup>; Geoff Davies<sup>1</sup>; Adam Senior<sup>1</sup>; Alan Edgington<sup>1</sup>; Rhys Jones<sup>1</sup>; Steve Plant<sup>1</sup>; Steve Jordan<sup>1</sup>; Claire Desbrow<sup>1</sup>; Paul Roberts<sup>1</sup>; Victor Vandell<sup>2</sup>; Elena Gairloch<sup>2</sup>; <sup>1</sup>*Biotage GB Limited, Cardiff, UK*; <sup>2</sup>*Biotage LLC, Charlotte, NC*
- WP 496 **Streamlined Method Development for Pharmacokinetic Analysis utilizing Robotic Sample Preparation and Ultra-fast SPE-MS/MS using a newly developed Triple Quadrupole MS**; Craig Love; Laura Pollum; Behrooz Zekavat; Patty Sun; Na Pi Parra; *Agilent Technologies, Inc, Santa Clara, CA*
- WP 497 **Compositional Analysis of Reverse Osmosis Membranes Post-Treated with Nitrous Acid**; Chengli Zu; Bruce Gerhart; Sam Qiu; Sarah LaFond; Jamie Stanley; Robert Cieslinski; *Dow Chemical Company, Midland, MI*
- WP 498 **Evaluating the Potential for Cross Contamination when Performing 96-Well Sample Preparation Prior to LC-MS/MS Analysis**; Helen Lodder<sup>1</sup>; Alan Edgington<sup>1</sup>; Lee Williams<sup>1</sup>; Geoff Davies<sup>1</sup>; Rhys Jones<sup>1</sup>; Adam Senior<sup>1</sup>; Steve Jordan<sup>1</sup>; Claire Desbrow<sup>1</sup>; Paul Roberts<sup>1</sup>; Victor Vandell<sup>2</sup>; Elena Gairloch<sup>2</sup>; <sup>1</sup>*Biotage GB Limited, Cardiff, UK*; <sup>2</sup>*Biotage LLC, Charlotte, NC*
- WP 499 **Gel-Aided Sample Preparation (GASP)—A Simplified Method for Gel-Assisted Proteomic Sample Generation from Protein Extracts and Intact Cells**; Roman Fischer; Benedikt Kessler; *University of Oxford, UK, Oxford, UK*
- WP 500 **The Effects of Heat Stabilization and Euthanasia Methods on Post-Sampling Release of Free Fatty Acids**; Fredrik Jernerén<sup>1</sup>; Marcus Söderquist<sup>2</sup>; Jörg Hanrieder<sup>3</sup>; Oskar Karlsson<sup>4,5</sup>; <sup>1</sup>*University of Oxford, Oxford, UK*; <sup>2</sup>*Denator, Uppsala, Sweden*; <sup>3</sup>*Chalmers Tech. University, Gothenburg, Sweden*; <sup>4</sup>*Uppsala University, Uppsala, Sweden*; <sup>5</sup>*Harvard University, Boston, MA*
- WP 501 **The Development of an Automated Online SPE-LC/MS/MS methodology for 25-OH-Vitamin D2, 25-OH-Vitamin D3 and 3-Epi-OH-Vitamin D3 in Human Serum**; Xianrong (Jenny) Wei; Sean Orłowicz; *Phenomenex, Torrance, CA*
- WP 502 **Evaluation of 25-hydroxy Vitamin D Extraction using Phospholipid Depletion Plate Technology and Method Comparison using Automated Sample Preparation**; Kerry Challenger<sup>1</sup>; Alan Edgington<sup>1</sup>; Lee Williams<sup>1</sup>; Helen Lodder<sup>1</sup>; Rhys Jones<sup>1</sup>; Geoff Davies<sup>1</sup>; Adam Senior<sup>1</sup>; Steve Jordan<sup>1</sup>; Claire Desbrow<sup>1</sup>; Paul Roberts<sup>1</sup>; Victor Vandell<sup>2</sup>;



- Elena Gairloch<sup>2</sup>; <sup>1</sup>Biotage GB Limited, Cardiff, UK; <sup>2</sup>Biotage LLC, Charlotte, NC
- WP 503 **Development of Novel On-line Rapid Solid Phase Extraction System for LC/HRMS Structural Analysis of Impurities using Nonvolatile Mobile Phases;** Ikuo Taoka<sup>1</sup>; Junetsu Igarashi<sup>1</sup>; Kazutoshi Matsuo<sup>2</sup>; <sup>1</sup>Sumitomo Dainippon Pharma Co., Ltd., Osaka, Japan; <sup>2</sup>Agilent Technologies, Osaka, Japan
- WP 504 **Automated Low Background Solid Phase Extraction System for Perfluorinated Compounds in Water;** Tom Hall; Justin Blau; *Fluid Management Systems, Watertown, MA*
- WP 505 **Analysis of Selected Drugs of Abuse in Human Urine with Automated Solid Phase Extraction and LC/MS;** Ryan Balgos; Tom Hall; *Fluid Management Systems, Watertown, MA*
- WP 506 **High Throughput Non-Depletive SPME Method for LC-MS/MS Simultaneous Determination of Free and Total Concentrations of Compounds with Varying Physicochemical Properties;** Ezel Boyaci; Barbara Bojko; Janusz Pawliszyn; *University of Waterloo, Waterloo, Canada*
- WP 507 **Automating Liquid-Liquid Extractions using an X-Y-Z Coordinate Autosampler for LC/MS/MS Analyses;** Fred Foster; John Stuff; Edward Pfannkoch; *Gerstel, Inc., Linthicum, MD*
- WP 508 **Bone Protein "Extract-omics": Comparing Extractions and Sub-Extractions for Mass Spectrometry Efficiency;** Elena Schroeter<sup>1</sup>; Caroline DeHart<sup>2</sup>; Mary Schweitzer<sup>1</sup>; Paul Thomas<sup>2</sup>; Neil Kelleher<sup>2</sup>; <sup>1</sup>North Carolina State University, Raleigh, NC; <sup>2</sup>Northwestern University, Evanston, IL
- WP 509 **An Efficient and Highly Improved Platform for Basic Reversed-Phase Off-Line Fractionation Enables Deep Proteome Coverage;** Dorte B. Bekker-Jensen; Tanveer Bath; Christian Kelstrup; Rosa Jersie-Christensen; Michael L. Nielsen; Jesper V. Olsen; *NNF Center for Protein Research, Copenhagen, Denmark*
- WP 510 **Rapid Antibody Digestion Enabled by a Sample Preparation Platform that Automates Reversed-Phase Cleanup and Digestion of Denatured Antibodies;** Steve Murphy; Michael Bovee; *Agilent Technologies, Madison, WI*
- WP 511 **Novel Titanium-doped Silica Material for Dispersive Solid Phase Extraction of Bovine Muscle and Human Blood Serum Matrices;** Bradley Vanmiddlesworth; John Hanrahan; *Glantrio Ltd, Cork, Ireland*
- WP 512 **Method Development for Glutathione Species Quantification in Blood and Saliva for Immune Health Assessment;** Patrick Benecewicz; H.M Skip Kingston; *Duquesne University, Pittsburgh, PA*
- WP 513 **Quantitative Peptide Assay for Optimized and Reproducible Sample Preparations for Mass Spectrometry Applications;** Xiaoyue Jiang<sup>1</sup>; Ramesh Ganapathy<sup>2</sup>; Sijian Hou<sup>2</sup>; Sergei Snovidia<sup>2</sup>; Ryan Bomgardner<sup>2</sup>; Paul Haney<sup>2</sup>; John Rogers<sup>2</sup>; Rosa Viner<sup>1</sup>; Andreas FR Huhmer<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific, Rockford, IL
- WP 514 **An Automated Sample Preparation System Based on the Mixing Driven by Oscillating Magnetic Fields;** Chang Liu<sup>1</sup>; Anne-Sophie Wavreille<sup>2</sup>; Jonathan Sidibe<sup>3</sup>; Gerard Hopfgartner<sup>3</sup>; Amar Rida<sup>2</sup>; J. Larry Campbell<sup>1</sup>; Don Arnold<sup>4</sup>; Tom Covey<sup>1</sup>; <sup>1</sup>SCIEX, Concord, ON, Canada; <sup>2</sup>Spinomix, Lausanne, Switzerland; <sup>3</sup>University of Geneva, Geneva, Switzerland; <sup>4</sup>Eksigent, part of SCIEX, Redwood City, CA
- WP 515 **An Analytical Evaluation Plasma Microsampling Capillaries – Effect of Thixotropic Gel and Stability of Analytes;** Kristen Jurusik<sup>1</sup>; Chester L Bowen<sup>1</sup>; Jim Kenney<sup>2</sup>; Joseph Siple<sup>2</sup>; <sup>1</sup>GlaxoSmithKline, King Of Prussia, PA; <sup>2</sup>Drummond Scientific, Broomall, PA
- WP 516 **Optimization of Automated High Throughput Trypsin Digests for Highly Reproducible Peptide Map Analysis;** Eric Johansen<sup>1</sup>; St John Skilton<sup>2</sup>; <sup>1</sup>SCIEX, Redwood City, CA; <sup>2</sup>SCIEX, Framingham, MA
- WP 517 **Surfactant-Assisted Extraction and Hydrophilic Interaction Liquid Chromatography/Mass Spectrometric Determination of Polar Vitamins from Biological Fluids;** Shining Lu; David Bell; *Sigma-Aldrich, Bellefonte, PA*
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- WP 518 **Creating Reproducible Micropatterned Analyte Surfaces to Investigate the Effect of Sample Preparation Parameters in the MALDI Imaging Mass Spectrometry Process;** Brian Malys; Abdirahman Abdillahi; Christopher Schultz; Kevin Owens; *Drexel University, Philadelphia, PA*
- WP 519 **High-resolution Ambient MS Imaging of Negative Ions in Positive Ion Mode: Using Dicationic Reagents for Surface Micro-Extraction with the Single-probe;** Wei Rao; Ning Pan; Zhibo Yang; *University of Oklahoma, Norman, OK*
- WP 520 **Creating Homogenous Matrix Coating for High Spatial Resolution (5 μm) Imaging MS;** Junhai Yang; Andre Zavalin; Lisa Manier; Paul Laibinis; Richard Caprioli; *Vanderbilt University, Nashville, TN*
- WP 521 **Rapid Pseudo-separations of Biological Samples Combined with MALDI Imaging;** Steve Bajic; Paul Murray; Mark Towers; *Waters Corporation, Wilmslow, UK*
- WP 522 **Enhanced MALDI MSI by *in situ* Tissue Lysis on Porous Silicon;** Adrien Mombrun<sup>1</sup>; Matthieu Dreyfus<sup>1</sup>; Céline Leclech<sup>1</sup>; Frederic-Xavier Gaillard<sup>1</sup>; Vera Aiello<sup>1</sup>; Laurent Selekt<sup>2</sup>; François Berger<sup>1,3</sup>; Ali Bouamrani<sup>1,3</sup>; <sup>1</sup>CEA-LETI Clinatex, Grenoble, France; <sup>2</sup>CHU-UJF, Grenoble, France; <sup>3</sup>INSERM Clinatex UA01, Grenoble, France
- WP 523 **Compound Stability Evaluation in Tissue Sections Determined Using Surface Sampling Micro-LC MS/MS;** Adam Bentley<sup>2</sup>; Christopher DeBenedetto<sup>2</sup>; Xiaojum Ren<sup>2</sup>; Vilmos Kertesz<sup>1</sup>; Paul Moench<sup>2</sup>; James Glick<sup>2</sup>; Robert Johnson<sup>2</sup>; Gary J. Van Berkel<sup>1</sup>; Jimmy Flaracos<sup>2</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>Novartis Institutes for Biomedical Research, East Hanover, NJ
- WP 524 **The Influence of Surface Permittivity and Sample Height on Mass Accuracy in MALDI-TOF Imaging;** Sophie Froehlich; Guenter Allmaier; Martina Marchetti-Deschmann; *Vienna University of Technology, Vienna, Austria*
- WP 525 **MALDI Imaging of On-Tissue Digests at High Spatial Resolution;** Shannon Cornett; *Bruker Daltonics, Billerica, MA*
- WP 526 **The Laser Desorption/Ionization Imaging Mass Spectrometry for Synthetic Polymer Analysis Assisted by Metal Nano-Particles;** Takaya Satoh<sup>1</sup>; Hironobu Niimi<sup>1</sup>; Makiko Fujii<sup>2</sup>; Toshio Seki<sup>2</sup>; Jiro Matsuo<sup>2</sup>; Masaaki Ubukata<sup>3</sup>; Robert DiPasquale<sup>3</sup>; <sup>1</sup>JEOL Ltd., Akishima, Japan; <sup>2</sup>Kyoto University, Kyoto, Japan; <sup>3</sup>JEOL USA Inc., Peabody, MA
- WP 527 **Sublimation of 6-aza-2-thiothymine: Development of an Imaging MS Method to Detect Glycolipids In Tissue Sections;** Kranjec Elizabeth-Ann; Pierre Chaurand; *University of Montreal, Montreal, Canada*
- WP 528 **Study of Experimental Conditions for MALDI Imaging by using Highly Controllable Sublimation Technique;** Takushi Yamamoto; Kaoru Kaneshiro; Yuzo Yamazaki; *Shimadzu Corporation, Kyoto, Japan*
- WP 529 **Gold Assisted LDI for High Resolution Imaging MS of Triacylglycerol from Thin Tissue Sections. Application to Alzheimer's disease;** Martin Dufresne; Laura Hamilton; Jean-François Masson; Karl Fernandes; Pierre Chaurand; *Université de Montréal, Montréal, Canada*
- WP 530 **Lipid Profiling of Formalin Fixed Tissues with DESI-MS Imaging, Eliminating the Requirement for Snap Freezing?** Emrys A Jones<sup>1</sup>; Jocelyn Tillner<sup>2</sup>; Mark Towers<sup>1</sup>; Emmanuelle Claude<sup>1</sup>; Zoltan Takats<sup>2</sup>; Jim Langridge<sup>1</sup>; <sup>1</sup>Waters Corporation, Wilmslow, UK; <sup>2</sup>Imperial College

- London, London, UK  
 WP 531 **GUMBOS and nanoGUMBOS as MALDI Imaging Matrix Compounds**; Hashim Alghafly; Tia Vargas; Kermit K. Murray; Isiah Warner; *Louisiana State University, Baton Rouge, LA*
- WP 532 **Matrix Optimization for the Analysis of Resin Acids and Lipids in Loblolly Pine Seedlings using MALDI-MSI**; Michelle Reid<sup>1</sup>; Rainey Patterson<sup>1</sup>; Gary F. Peter<sup>2</sup>; Richard A. Yost<sup>1</sup>; <sup>1</sup>*Chemistry Department, University of Florida, Gainesville, FL*; <sup>2</sup>*Genetics Institute, University of Florida, Gainesville, FL*
- IMAGING MS: METHOD DEVELOPMENT I**  
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- WP 533 **Development of Saponification Approach for MALDI Mass Spectrometry Imaging**; Maomao Zeng; Stanislav S. Rubakhin; Jonathan V. Sweedler; *University of Illinois, Urbana, Illinois*
- WP 534 **Large Scale MALDI-MS Imaging of a Germinated Corn Seed: Toward Mass Spectrometry Imaging of Plant Metabolome**; Adam Feenstra<sup>1,2</sup>; Young Jin Lee<sup>1,2</sup>; <sup>1</sup>*Iowa State University, Ames, IA*; <sup>2</sup>*Ames Laboratory-USDOE, Ames, IA*
- WP 535 **In situ Top Down Proteomics: Targeted Imaging of Histones in Tissue Using Laser Ablation Electrospray Ionization Mass Spectrometry (LAESI-MS)**; Pamela Cantrell; Peggi Angel; Callee Walsh; *Protea Biosciences, Inc., Morgantown, WV*
- WP 536 **Towards High Resolution Quantitative Chemical Imaging: Combining SRS and MALDI**; Elizabeth Randall<sup>1</sup>; Alasdair Rae<sup>2</sup>; Rory Steven<sup>2</sup>; Alan Race<sup>2</sup>; Helen Cooper<sup>1</sup>; Iain Styles<sup>1</sup>; Josephine Bunch<sup>2,3</sup>; <sup>1</sup>*University of Birmingham, Birmingham, UK*; <sup>2</sup>*The National Physical Laboratory, Teddington, UK*; <sup>3</sup>*University of Nottingham, Nottingham, UK*
- WP 537 **Molecular Imaging of Protein in Tissues Using Ambient Ionization Top-Down Mass Spectrometry**; Cheng-Chih Hsu<sup>1,2</sup>; Qianhao Min<sup>1,3</sup>; Livia Eberlin<sup>1</sup>; Richard Zare<sup>1</sup>; <sup>1</sup>*Stanford University, Stanford, CA*; <sup>2</sup>*National Taiwan University, Taipei, Taiwan*; <sup>3</sup>*Nanjing University, Nanjing, China*
- WP 538 **A New Vacuum Stable Matrix for High-Speed 3D MALDI Image Acquisition**; Wesley Bryson<sup>1</sup>; Jeffrey Spraggins<sup>1</sup>; Raf Van De Plas<sup>2</sup>; Shannon Cornett<sup>3</sup>; Richard Caprioli<sup>1</sup>; <sup>1</sup>*Vanderbilt University, Nashville, TN*; <sup>2</sup>*Delft University of Technology, Delft, Netherlands*; <sup>3</sup>*Bruker Daltonics Inc., Billerica, MA*
- WP 539 **An Optimized IMS Data Protocol to Assess the Changes in the Lipidome of Xenografts After Administration of 2-Hydroxyoleic Acid**; Roberto Fernández<sup>1</sup>; Jone Garate<sup>1</sup>; Sergio Lage<sup>1</sup>; Silvia Terés<sup>2</sup>; Monica Higuera<sup>3</sup>; Joan Bestard-Escalas<sup>4</sup>; Daniel Horacio Lopez<sup>4</sup>; Francisca Guardiola<sup>3</sup>; Pablo V. Escribá<sup>3</sup>; Gwendolyn Barceló-Coblijn<sup>4</sup>; José Andrés Fernández<sup>1</sup>; <sup>1</sup>*University of Basque Country, UPV/EHU, Leioa, Basque Country, Spain*; <sup>2</sup>*Institut européen de chimie et biologie, Pessac, France*; <sup>3</sup>*University of the Balearic Islands, Palma, Balearic Islands, Spain*; <sup>4</sup>*Palma Health Research Institute, Palma, Balearic Islands, Spain*
- WP 540 **Top-Down Protein Identification from Tissue Sections by Microproteomics Approach**; Vivian Delcourt<sup>1,2</sup>; Julien Franck<sup>1</sup>; Jusal Quanico<sup>1</sup>; Maxence Wisztorski<sup>1</sup>; Xavier Roucou<sup>2</sup>; Michel Salzet<sup>1</sup>; Isabelle Fournier<sup>1</sup>; <sup>1</sup>*University Lille1, Villeneuve d'Ascq, France*; <sup>2</sup>*University of Sherbrooke, Sherbrooke, Quebec, Canada*
- WP 541 **Multiplexed TOF/TOF Analysis in a Single Laser Shot for Improved Quantification and Applications to MALDI Imaging Mass Spectrometry**; Boone Prentice<sup>1</sup>; Chad Chumbley<sup>2</sup>; Brian Hachey<sup>1</sup>; Jeremy L. Norris<sup>1</sup>; Richard Caprioli<sup>1,2</sup>; <sup>1</sup>*Vanderbilt University School of Medicine, Nashville, TN*; <sup>2</sup>*Vanderbilt University, Nashville, TN*
- WP 542 **An Integrated and High Throughput Approach for in situ Protein Digestion, Peptide Imaging and Sequence Verification**; Fengfei Ma; Jingxin Wang; Lingjun Li; *Univ of Wisconsin-Madison, Madison, WI*
- WP 543 **De novo Discovery of Tumor Clones Linked to Metastasis and Poor Prognosis Using MALDI Imaging Mass Spectrometry**; Benjamin Balluff<sup>1</sup>; Walid Abdelmoula<sup>1</sup>; Jouke Dijkstra<sup>1</sup>; Axel Walch<sup>2</sup>; Liam McDonnell<sup>3</sup>; <sup>1</sup>*LUMC, Leiden, NL*; <sup>2</sup>*Helmholtz Zentrum München, Munich, DE*; <sup>3</sup>*LUMC & PSF, Pisa, Italy*
- WP 544 **Contrast-Enhanced Mass Spectrometry Imaging Reveals Tumour Heterogeneity and Boundaries**; Alessandra Tata<sup>1,2</sup>; Jinzi Zheng<sup>2</sup>; Howard Ginsberg<sup>3</sup>; David Jaffray<sup>2,4</sup>; Demian Iffa<sup>1</sup>; Arash Zarrine Afsar<sup>2,3</sup>; <sup>1</sup>*Department of Chemistry, CRMS, York University, Toronto, Canada*; <sup>2</sup>*Techna, University Health Network, Toronto, Canada*; <sup>3</sup>*Dept. of Surgery, University of Toronto, Toronto, Canada*; <sup>4</sup>*Dept. Medical Biophysics, University of Toronto, Toronto, Canada*
- WP 545 **New Biomarkers Discovery Approach based on Morphological Evaluation of Mass Spectrometry Imaging (MSI) Dataset: A Case Study**; Gael Picard de Muller; Gregory Hamm; Fabien Pamelard; David Bonnel; Kevin Lorgouilloux; Jonathan Stauber; *ImaBiotech, MS Imaging Dept., Loos, France*
- WP 546 **Mass Spectrometry Imaging of Proteins after On-Tissue Digestion: Approaching Cellular Resolution in Fresh-Frozen and FFPE Tissue**; Andreas Roempp; Katharina Huber; Pegah Khamsehgir-Silz; Bernhard Spengler; *Justus Liebig University, Giessen, Germany*
- WP 547 **In situ Assaying the Activity of Ammonia Lyase Mutants Demonstrated by a Bi-Substrate Model Reaction with DESI IM MS Imaging**; Cunyu Yan<sup>1</sup>; Fabio Parmeggiani<sup>1</sup>; Jason Schmidberger<sup>1</sup>; Emrys Jones<sup>2</sup>; Emmanuelle Claude<sup>2</sup>; Nicholas J. Turner<sup>1</sup>; Sabine L. Flitsch<sup>1</sup>; Perdita Barran<sup>1</sup>; <sup>1</sup>*University of Manchester, Manchester, UK*; <sup>2</sup>*Waters MS Technologies Centre, Wilmslow, UK*
- WP 548 **Examination of Plasmodium berghei Oocysts in the Mosquito using MALDI Fourier Transform Imaging Mass Spectrometry**; Berin Boughton<sup>1</sup>; Daniel Sarabia<sup>2</sup>; Dean Goodman<sup>2</sup>; Mark Condina<sup>3</sup>; Geoff McFadden<sup>2</sup>; Ute Roessner<sup>2</sup>; <sup>1</sup>*Metabolomics Australia, University of Melbourne, Parkville, Australia*; <sup>2</sup>*School of Biosciences, The University of Melbourne, Parkville, VIC, Australia*; <sup>3</sup>*Bruker Pty Ltd, Melbourne, VIC, Australia*
- WP 549 **An Investigation into Multi-Model Tissue Imaging on a Single Section by DESI and MALDI TOF Mass Spectrometry**; Mark Towers<sup>1</sup>; Emrys Jones<sup>1</sup>; Anna Mroz<sup>2</sup>; Zoltan Takats<sup>2</sup>; Emmanuelle Claude<sup>1</sup>; Jim Langridge<sup>1</sup>; <sup>1</sup>*Waters Corporation, Wilmslow, UK*; <sup>2</sup>*Imperial College London, London, UK*
- WP 550 **Visualization of Lipids Involved in the Growth of Pseudomonas putida Biofilm using Matrix-Assisted Laser Desorption Ionization Mass Spectrometry Imaging**; Bin Li<sup>1</sup>; Sage Dunham<sup>1</sup>; Travis King<sup>2</sup>; Kensey R. Amaya<sup>2</sup>; Jonathan Sweedler<sup>1</sup>; <sup>1</sup>*University of Illinois at Urbana-Champaign, Urbana, IL*; <sup>2</sup>*ERDC-CERL, Environmental Chemistry Laboratory, Champaign, IL*
- WP 551 **A Comprehensive Study of the Brain Lipidome Using Silver Nanoparticles (Colloidal and Implanted)**; Ludovic Muller<sup>1</sup>; Aurelie Roux<sup>1</sup>; Shelley N Jackson<sup>1</sup>; J. Albert Schultz<sup>2</sup>; Amina S. Woods<sup>1</sup>; <sup>1</sup>*NIH/NIDA-IRP, Baltimore, MD*; <sup>2</sup>*Ionwerks, Houston, TX*
- WP 552 **Enhancing in situ Biomolecule Identification by Novel Combination of Multiplexed Mass Spectrometric Imaging with DDA on a MALDI Orbitrap Platform**; Chuanzi OuYang<sup>1</sup>; Bingming Chen<sup>2</sup>; Lingjun Li<sup>1,2</sup>; <sup>1</sup>*Department of Chemistry, UW-Madison, Madison, WI*; <sup>2</sup>*School of Pharmacy, UW-Madison, Madison, WI*
- WP 553 **Advanced Multi-modal Mass Spectrometry Applied to the Complexity of Lipid Imaging Analysis**; Katherine Kellersberger; Shannon Cornett; Michael Easterling; *Bruker Daltonics, Billerica, MA*





- WP 554 **Molecular Mapping of Alzheimer's Disease – Imaging Mass Spectrometry**; [Andrea Kelley](#)<sup>1</sup>; George Perry<sup>1</sup>; Rudolph J. Castellani<sup>2</sup>; Stephan Bach<sup>1</sup>; <sup>1</sup>University of Texas at San Antonio, San Antonio, Tx; <sup>2</sup>University of Maryland School of Medicine, Baltimore, MD
- ION MOBILITY: STRUCTURES**  
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- WP 555 **Understanding the Roles of Electronic and Steric Effects in Separating Isomers using Differential Mobility Spectrometry**; [Chris J. Lock](#)<sup>1</sup>; J. Larry Campbell<sup>1</sup>; Chang Liu<sup>1</sup>; J.C. Yves Leblanc<sup>1</sup>; Jeffrey Shields<sup>2</sup>; John Janiszewski<sup>2</sup>; Christian Ieritano<sup>3</sup>; Gene Ye<sup>3</sup>; Gillian Hawes<sup>3</sup>; Moaraj Hasan<sup>3</sup>; W. Scott Hopkins<sup>3</sup>; <sup>1</sup>SCIEX, Concord, ON, Canada; <sup>2</sup>Pfizer, Groton, CT; <sup>3</sup>University of Waterloo, Waterloo, ON, Canada
- WP 556 **Characterizing Biomolecular Ion Structure using Ion Mobility Spectrometry Coupled with Gas-Phase Hydrogen Deuterium Exchange And Tandem Mass Spectrometry**; [Stephen Valentine](#); Mahdiar Khakinejad; Samaneh Ghassabi-Kondalaji; Gregory Donohoe; Jim Arndt; West Virginia University, Morgantown, WV
- WP 557 **Ion Mobility Spectrometry of Foldamers: Characterization of the Folding State**; [Frederic Rosu](#)<sup>1,2</sup>; Xuesong Li<sup>1,3</sup>; Victor Maurizot<sup>1,3</sup>; Ivan Huc<sup>1,3</sup>; Valerie Gabelica<sup>1,4</sup>; <sup>1</sup>Univ. Bordeaux, IECB, Bordeaux, France; <sup>2</sup>CNRS UMS 3033, IECB, Pessac, France; <sup>3</sup>CNRS UMR 5284, CBMN, Pessac, France; <sup>4</sup>INSERM, U869, ARNA Laboratory, Bordeaux, France
- WP 558 **Effect of Temperature, Charge, and Time on the Electrical Mobility of Minimally Perturbed Electro sprayed Protein Ions in the Gas Phase**; Michel Attoui<sup>1</sup>; [Juan Fernandez de la Mora](#)<sup>2</sup>; <sup>1</sup>Physics Department, University of Paris 12, Paris, France; <sup>2</sup>Yale University - Mechanical Engineering Department, New Haven, CT
- WP 559 **What Happens to DNA Duplexes in the Gas Phase?** Massimiliano Porrini<sup>1,2</sup>; Frederic Rosu<sup>3</sup>; [Valerie Gabelica](#)<sup>1,2</sup>; <sup>1</sup>University of Bordeaux, IECB, Pessac, France; <sup>2</sup>INSERM, U869, ARNA laboratory, Bordeaux, France; <sup>3</sup>CNRS, UMS 3033, IECB, University of Bordeaux, Pessac, France
- WP 560 **Ion Mobility Quadrupole Time-of-Flight (IM Q-TOF) Mass Spectrometric Applications of Monoclonal Antibody and its Derivatives**; David Wong; [Agilent Technologies, Inc.](#), Santa Clara, CA
- WP 561 **The Influence of Lipid Bilayer Physicochemical Properties on the Conformer Preferences of the Model Ion Channel Gramicidin A**; [John Patrick](#)<sup>1,2</sup>; David H. Russell<sup>1,2</sup>; <sup>1</sup>Texas A&M University, College Station, TX; <sup>2</sup>Texas A&M University, College Station, TX
- WP 562 **Conformational Landscapes of Model Proteins Measured on a Commercial Drift Tube Ion Mobility-Mass Spectrometer**; [Ewa Jurneczko](#)<sup>1</sup>; Jody C. May<sup>1</sup>; George C. Stafford<sup>2</sup>; John C. Fjeldsted<sup>2</sup>; John A. McLean<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, Tennessee; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- WP 563 **On the Role of Penultimate Proline Isomerizations in Neuropeptide Conformations**; [Matthew Glover](#); David Clemmer; Indiana University, Bloomington, IN
- WP 564 **Ion Mobility Mass Spectrometry as a Tool to Perform Structural Characterization of Peptides Bearing Disulfide Bond(s)**; [Philippe Massonnet](#)<sup>1</sup>; Gregory Uper<sup>2</sup>; Michel Degueldre<sup>1</sup>; Denis Morsa<sup>1</sup>; Nicolas Smargiasso<sup>1</sup>; Nicolas Gilles<sup>2</sup>; Loic Quinton<sup>1</sup>; Edwin De Pauw<sup>1</sup>; <sup>1</sup>Laboratory of Mass Spectrometry - Ulg, Liège, Belgium; <sup>2</sup>CEA/DSV/ iBiTec-S/SIMOPRO, Gif sur Yvette, France
- WP 565 **Extracting Collision Cross-sections of Ion Mobility Unresolved Isomers Using Tandem Mass Spectrometry and Chemometric Deconvolution**; [Brett Harper](#); Elizabeth Neumann; Touradj Solouki; Baylor University, Waco, TX
- WP 566 **The Role of Inter- and Intramolecular Interactions on the Conformer Preferences of Biomolecules during Electrospray Ionization**; [Kelly Servage](#)<sup>1</sup>; Joshua Silveira<sup>2</sup>; Kyle Fort<sup>3</sup>; David H. Russell<sup>1</sup>; <sup>1</sup>Texas A&M University, College Station, TX; <sup>2</sup>Bruker Daltonics, Billerica, MA; <sup>3</sup>Utrecht University, CH Utrecht, The Netherlands
- WP 567 **Correlating Ion-Neutral Collision Cross Sections to Protein Native Conformation and Energy Folding Landscape**; Shu-Hua Chen; [David H. Russell](#); Texas A&M University, College Station, TX
- WP 568 **Investigation of Ion Mobility Mass Spectrometry Analysis of Electrochemically Generated Oxidation Products of Opiates and Comparison with Theoretical CCS Values**; Cris Laphorn<sup>1</sup>; Frank Pullen<sup>1</sup>; Susana da Silva Torres<sup>2</sup>; Mark R. Taylor<sup>2</sup>; Russell Mortishire-Smith<sup>3</sup>; [Jayne Kirk](#)<sup>3</sup>; Andrew Baker<sup>4</sup>; <sup>1</sup>University of Greenwich, Chatham Maritime, UK; <sup>2</sup>Pfizer, Sandwich, UK; <sup>3</sup>Waters Corp, Manchester, UK; <sup>4</sup>Waters, Inc., Pleasanton, CA
- WP 569 **Ion Mobility - Mass Spectrometry for Structural Analysis of Protein Therapeutics**; [Carly Ferguson](#); Michael Boyne; Ashley Gucinski; Food and Drug Administration, St. Louis, MO
- WP 570 **Changes in Drift Spectra Intensity Distribution of Cyclodextrin Negative Ions with Solution pH**; Paul S. Blank<sup>1</sup>; Christian Klein<sup>2</sup>; Julie Wight<sup>3</sup>; Ruwan Kurulugama<sup>2</sup>; Stephanie Cologna<sup>1</sup>; Peter S. Backlund<sup>1</sup>; [Alfred L. Yergey](#)<sup>1</sup>; <sup>1</sup>NIH, Bethesda, MD; <sup>2</sup>Agilent Technologies, Santa Clara, CA; <sup>3</sup>Agilent Technologies, Poolesville, MD
- WP 571 **Protein Structure Collapse in the Gas-phase Revealed by Ion Mobility and Molecular Dynamics**; [Iain D.G. Campuzano](#)<sup>1</sup>; Morgan Lawrenz<sup>1</sup>; Carlos Larriba Andaluz<sup>2</sup>; <sup>1</sup>Amgen Inc., Thousand Oaks, CA; <sup>2</sup>University of Minnesota, Bloomington, IN
- WP 572 **Probing Solution-Related Structures of Disordered Peptide Indolicidin with IMS-MS and IMS-IMS-MS Techniques**; [Neelam Khanal](#); Maissa M. Gaye; David E. Clemmer; Department of Chemistry, Indiana University, Bloomington, IN
- WP 573 **Electrospray Ionization of Proteins: Conformations Versus Aggregates Probed by Ion Mobility/Mass Spectrometry**; [Kent Gillig](#); Chung-Hsuan Chen; Academia Sinica, Taipei, Taiwan
- WP 574 **Effect of beta-Cyclodextrin on Protein Structure Investigated by Ion Mobility-Mass Spectrometry**; Yinjuan Chen<sup>1</sup>; [Xinhua Dai](#)<sup>2</sup>; Peng Xiao<sup>2</sup>; Xiang Fang<sup>2</sup>; Chuan-Fan Ding<sup>1</sup>; <sup>1</sup>Fudan University, Shanghai, China; <sup>2</sup>National Institute of Metrology, Beijing, China
- WP 575 **Evidence for Differential Structural Preferences of the Leu7Pro Mutant Neuropeptide Y Signal Peptide Probed by Ion Mobility-Mass Spectrometry**; [Zhengwei Chen](#); Christopher Lietz; Lingjun Li; University of Wisconsin-Madison, Madison, WI
- ION MOBILITY: NON-COVALENT COMPLEXES**  
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- WP 576 **Investigating Changes in the Gas-Phase Conformation of Heparin/HS binding Proteins Using Traveling Wave Ion Mobility Spectrometry (TWIMS)**; [Yuejie Zhao](#)<sup>1</sup>; Lingyun Li<sup>2</sup>; Robert Linhardt<sup>2</sup>; Yongmei Xu<sup>3</sup>; Jian Liu<sup>3</sup>; Arunima Singh<sup>1</sup>; Robert Woods<sup>1</sup>; Jon Amster<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA; <sup>2</sup>Rensselaer Polytechnic University, Troy, NY; <sup>3</sup>University of North Carolina, Chapel Hill, NC
- WP 577 **Utilizing High Throughput IMS-MS Measurements to Study Noncovalent Protein/Ligand Interactions Kinetics**; [Daniel J. Orton](#)<sup>1</sup>; Ryan T. Kelly<sup>2</sup>; Yehia M. Ibrahim<sup>1</sup>; Xing Zhang<sup>1</sup>; Tridib Ghosh<sup>2</sup>; John R. Cort<sup>1</sup>; Richard D. Smith<sup>1</sup>; Erin S. Baker<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>Environmental Molecular Sciences Laboratory PNNL, Richland, WA
- WP 578 **Application of Ion Mobility Mass Spectrometry for the Analysis of Ruthenium-Arene Complexes**; [Izabella Czerwinska](#); Johann Far; Christopher Kune;



Nicolas Smargiasso; Denis Morsa; Edwin De Pauw; *Mass Spectrometry Laboratory, GIGA-R, University of Liege, Belgium*

- WP 579 **Evaluating Ion Mobility-Mass Spectrometry as a Tool for Discovering Conformationally-Selective Src Kinase Inhibitors;** [Jessica Rabuck-Gibbons](#); Matthew Soellner; Brandon Ruotolo; *University of Michigan, Ann Arbor, MI*
- WP 580 **Mass and Mobility Distributions of Labile Metal Complexes of Uranium, Barium, Cesium and Lanthanum;** [Austen Davis](#); Brian H. Clowers; *Washington State University, Pullman, WA*
- WP 581 **Ion Mobility-Mass Spectrometry for Screening Libraries of Rationally-designed Bifunctional Small Molecule Libraries Capable of Chemical and Structural Amyloid Modulation;** [Richard A. Kerr](#)<sup>1</sup>; Younwoo Nam<sup>2</sup>; Michael Beck<sup>1</sup>; Mi Hee Lim<sup>2</sup>; Brandon T. Ruotolo<sup>1</sup>; *<sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>Ulsan National Institute of Science and Technology, Ulsan, South Korea*
- WP 582 **Ion Mobility Mass Spectrometry: A New Approach for Polymer Drug Carrier and Delivery Characterization;** [Jean R. N. Haler](#)<sup>1,2</sup>; Denis Morsa<sup>1</sup>; Johann Far<sup>1</sup>; Philippe Lecomte<sup>2</sup>; Christine Jérôme<sup>2</sup>; Edwin De Pauw<sup>1</sup>; *<sup>1</sup>Mass Spectrometry Laboratory, University of Liège, Liège, Belgium; <sup>2</sup>CERM, University of Liège, Liège, Belgium*
- WP 583 **Neuropeptide Inspired Alzheimer's Disease Therapeutic Discovery Utilizing Ion Mobility - Mass Spectrometry;** [Molly Soper](#); Brandon Ruotolo; *University Of Michigan, Ann Arbor, MI*
- WP 584 **A Collision Induced Unfolding Assay for differentiating ATP-competitive and Allosteric Protein Tyrosine Kinase Inhibitors;** [James Keating](#); [Jessica Rabuck-Gibbons](#); Brandon Ruotolo; *University of Michigan, Department of Chemistry, Ann Arbor, MI*
- WP 585 **Ion Mobility-Mass Spectrometry Reveals the Early Assembly of Amyloid  $\beta$ -protein: The effects of Familial Mutations A2T and A2V;** [Xueyun Zheng](#)<sup>1</sup>; Robin Roychoudhuri<sup>2</sup>; David Teplow<sup>2</sup>; Michael T. Bowers<sup>1</sup>; *<sup>1</sup>University of California, Santa Barbara, CA; <sup>2</sup>University of California, Los Angeles, CA*
- WP 586 **Effect of Glycosaminoglycan Disaccharide Binding on the Structural Heterogeneity and Dynamics of the Chemokine CCL5;** [Hiroki Sakai](#); Christian Bleiholder; *Florida State University, Tallahassee, FL*

**PROTEINS: NON-COVALENT INTERACTIONS**  
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- WP 587 **Monitoring Protein Stabilization by Multiple Analytical Techniques;** [Krishnamoorthy Kuppannan](#)<sup>1</sup>; Margaret Covington<sup>1</sup>; Florin Dan<sup>1</sup>; Yujing Tan<sup>1</sup>; Yongfu Li<sup>1</sup>; David Meunier<sup>1</sup>; Danielle Dodge<sup>1</sup>; Joshua Katz<sup>2</sup>; *<sup>1</sup>The Dow Chemical Company, Midland, MI; <sup>2</sup>The Dow Chemical Company, Collegeville, PA*
- WP 588 **Multisubunit Protein Interactions and Protein-Ligand Binding Sites Revealed By Surface Induced Dissociation Ion Mobility-Mass Spectrometry;** [Yue Ju](#); Royston Quintyn; Vicki Wysocki; *The Ohio State University, Columbus, Ohio*
- WP 589 **Screening Glycolipids Against Proteins using Electrospray Ionization Mass Spectrometry and Picodiscs;** [Jun Li](#); Elena Kitova; John Klassen; *University of Alberta, Edmonton, Canada*
- WP 590 **The GFP Interactome: Implications for Assessing GFP-tagged Protein Interactions using Immunoaffinity Purification-Mass Spectrometry Analysis;** Tara Nash; Kevin Blackburn; Steven Clouse; [Michael Goshe](#); *North Carolina State University, Raleigh, NC*
- WP 591 **Native nano-ESI-MS Application in Fragment Based Drug Discovery: Investigating Antagonism of Protein-Protein Interactions;** [Agni Faviola Mika Gavriilidou](#)<sup>1</sup>; Finn Holding<sup>2</sup>; Renato Zenobi<sup>1</sup>; *<sup>1</sup>ETH, Department of Chemistry*

& Applied Biosciences, Zurich, Switzerland; <sup>2</sup>Astex Pharmaceuticals, Cambridge, UK

- WP 592 **Enhanced I-DIRT (el-DIRT): Improved Identification of Specific Protein-Protein Interactions in Cellular Milieus by Glutaraldehyde Stabilization and Stable Isotope Labeling MS;** [Roman Subbotin](#); Julio Padovan; Brian Chait; *The Rockefeller University, New York, NY*
- WP 593 **Quantifying Protein-Glycolipid Interactions in Different Lipid Environments using Electrospray Ionization Mass Spectrometry;** [Ling Han](#); Elena Kitova; John Klassen; *University of Alberta, Edmonton, Canada*
- WP 594 **Protein-Protein Interaction (PPI) In Lectin Affinity Chromatography;** Jihoon Shin<sup>1</sup>; [Youngwon Jung](#)<sup>2</sup>; Wonryeon Cho<sup>1</sup>; *<sup>1</sup>Wonkwang University, Iksan, Republic of Korea; <sup>2</sup>Yonsei University, Seoul, Republic of Korea*
- WP 595 **Use of Native Mass Spectrometry for Quantification of Protein Complex;** [Wenjing Li](#); Bao Tran; Sung Hwan Yoon; Keely Pierzchalski; Jianshi Yu; David R Goodlett; Maureen A Kane; *University of Maryland, Baltimore, MD*
- WP 596 **Mutual Stabilization of Helix Structures in the Three-Helix Bundle Protein KIX Studied by Electron Capture Dissociation;** [Eva-Maria Schneeberger](#); Moritz Schennach; Kathrin Breuker; *University of Innsbruck, Innsbruck, Austria*
- WP 597 **Epitope Mapping of West Nile Virus Envelope Protein Bound to a Therapeutic Antibody by FPOP and HDX: Method Development;** [Yining Huang](#)<sup>1</sup>; Manolo Plasencia<sup>1</sup>; Melissa A. Edeling<sup>2</sup>; Christopher A. Nelson<sup>2</sup>; Don L. Rempel<sup>1</sup>; Henry W. Rohrs<sup>1</sup>; Daved H. Fremont<sup>2</sup>; Michael L. Gross<sup>1</sup>; *<sup>1</sup>Washington University in St. Louis, St. Louis, MO; <sup>2</sup>Washington University School of Medicine, St. Louis, MO*
- WP 598 **193nm UVPD of Natively Ionized DHFR for Elucidation of Protein-Ligand Interactions and Conformational Movements upon Inhibition by Methotrexate;** [Michael Cammarata](#); Ross Thyer; Jennifer Brodbelt; *The University of Texas, Austin, TX*
- WP 599 **Epitope Mapping of WNV Envelope Protein Bound to a Therapeutic Antibody by FPOP: Correlation of Interface Dynamics and Oxidative Labeling;** [Manolo Plasencia](#)<sup>1</sup>; Yining Huang<sup>1</sup>; Melissa A. Edeling<sup>2</sup>; Christopher A. Nelson<sup>2</sup>; Don L. Rempel<sup>1</sup>; Henry W. Rohrs<sup>1</sup>; Daved H. Fremont<sup>2</sup>; Michael L. Gross<sup>1</sup>; *<sup>1</sup>Washington University in St. Louis, St. Louis, MO; <sup>2</sup>Washington University School of Medicine, St. Louis, MO*
- WP 600 **Tannins (Procyanidins) Binding to a Salivary Peptide (Histatin 5) Studied using Electrospray Ionization Tandem Mass Spectrometry (ESI-MS/MS) and Molecular Simulations;** Joshua M. Shraberg<sup>1</sup>; Steven W. Rick<sup>1</sup>; Nalaka Rannulu<sup>1</sup>; [Richard B. Cole](#)<sup>1,2</sup>; *<sup>1</sup>Dept. Of Chemistry, U. Of New Orleans, New Orleans, LA; <sup>2</sup>Univ. P. et M. Curie (Paris 6), Paris Cedex 05, France*
- WP 601 **Determining the Cooperativity and Structural Effects of Copper Binding to the Homotetramer CsoR;** [Alexander D. Jacobs](#)<sup>1</sup>; Feng-Ming Chang<sup>1</sup>; Lindsay J. Morrison<sup>2</sup>; Jonathan M. Dilger<sup>1</sup>; Vicki H. Wysocki<sup>2</sup>; David P. Giedroc<sup>1</sup>; David E. Clemmer<sup>1</sup>; *<sup>1</sup>Indiana University, Bloomington, IN; <sup>2</sup>Ohio State University, Columbus, OH*
- WP 602 **Drugging the Undruggable: IM-MS Functional Binding Assay for Small Molecule Inhibitors of Conformationally Dynamic Proteins;** [Chris Nortcliffe](#)<sup>1</sup>; Giovanna Zinzalla<sup>2</sup>; Perdita Barran<sup>1</sup>; *<sup>1</sup>University of Manchester, Manchester, UK; <sup>2</sup>Karolinska Institutet, Stockholm, Sweden*
- WP 603 **Protein Interaction Partners of Protein Phosphatase 2A Catalytic Subunit in Rat  $\beta$ -Islet cells Using Quantitative Mass Spectrometry;** [Divyasri Damacharla](#); xiangmin Zhang; Danjun Ma; Yue Qi; Anjaneyulu Kowluru; Zhengping Yi; *Wayne State University, Detroit, MI*
- WP 604 **Combining Native MS and IM-MS for Structural Elucidation of the yeast mRNA 3'-end Maturation Complex CFIA;** [Johann Stojko](#)<sup>1</sup>; Adrien Dupin<sup>2</sup>; Sébastien



Fribourg<sup>2</sup>; Alain Van Dorsselaer<sup>1</sup>; Sarah Cianféran<sup>1</sup>;  
<sup>1</sup>LSMBO, DSA, IPHC, Strasbourg, France; <sup>2</sup>INSERM, U869,  
 IECB, Bordeaux, France

### STRUCTURAL BIOLOGY 605-617

- WP 605 **Allosteric Activation of Tumor Suppressor PP2A by a Small Molecule Activator Series Revealed using Hydroxyl Radical Footprinting**; Janna Kiselar<sup>1</sup>; Giri Gokulrangan<sup>2</sup>; David Kastrinsky<sup>3</sup>; Nilesh Zaware<sup>3</sup>; Michael Ohlmeyer<sup>3</sup>; Mark R Chance<sup>1</sup>; Goutham Narla<sup>1</sup>;  
<sup>1</sup>Case Western Reserve Univ, Cleveland, OH; <sup>2</sup>Pfizer Biotherapeutics WRD, Andover, MA; <sup>3</sup>Mount Sinai Hospital, NY, NY
- WP 606 **Structural and Biochemical Characterisation of Oligomeric Alpha-Synuclein by Ion Mobility Spectrometry - Mass Spectrometry**; Eva Illes-Toth<sup>2</sup>; Mafalda Ramos<sup>2</sup>; Roberto Cappai<sup>1</sup>; Caroline Dalton<sup>2</sup>; David Smith<sup>2</sup>;  
<sup>1</sup>University of Melbourne, Melbourne, VIC; <sup>2</sup>Sheffield Hallam University, Sheffield, UK
- WP 607 **Probing Ligand Interactions of the Chemokine Receptor CXCR7 by Mass Spectrometry**; Liwen Wang<sup>1</sup>; Martin Gustavsson<sup>2</sup>; Tracy Handel<sup>2</sup>; Mark R. Chance<sup>1</sup>;  
<sup>1</sup>Case Western Reserve Univ, Cleveland, OH; <sup>2</sup>University of California, San Diego, San Diego, CA
- WP 608 **Charge Detection Mass Spectrometry Measures DNA Packaging in Bacteriophage P22 above 50 MDa and Resolves Four Morphologies in Mutant P22**; David Keifer<sup>1</sup>; Kevin Bond<sup>1</sup>; Martin Jarrold<sup>1</sup>;  
 Indiana University, Bloomington, IN
- WP 609 **A Hybrid MS-based Strategy Provides Structural Insights into Transient Protein Assemblies**; Argyris Politis<sup>1</sup>;  
 King's College London, London, UK
- WP 610 **Exploring the Protein-Protein Chemical Crosslinking of a Highly Non-Iso-Stoichiometric Protein Complex**; Yeva Mirzakhanyan<sup>1</sup>; Tuan ngo<sup>1</sup>; Paul Gershon<sup>1</sup>;  
 UC-Irvine, Irvine, CA
- WP 611 **Molecular Architecture of the Yeast Mediator Complex**; Michael Trnka<sup>1</sup>; Philip Robinson<sup>2</sup>; Riccardo Pellarin<sup>1</sup>; Sali Andrej<sup>1</sup>; Roger Kornberg<sup>2</sup>; AL Burlingame<sup>1</sup>;  
<sup>1</sup>University of California, San Francisco, San Francisco, CA; <sup>2</sup>Stanford University, Stanford, CA
- WP 612 **A Structural Proteomics Study of High-Density Lipoprotein (HDL)**; Jason Serpa<sup>1</sup>; Teddy Chan<sup>2</sup>; Gordon Francis<sup>2</sup>; Evgeniy Petrotchenko<sup>1</sup>; Christoph Borchers<sup>1,3</sup>;  
<sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada; <sup>2</sup>Ctr. for Heart Lung Innov., UBC & St. Paul's Hosp., Vancouver, BC, Canada; <sup>3</sup>Dept. of Biochem. & Microbiol., Univ. of Victoria, Victoria, BC, Canada
- WP 613 **Probing Intact Red Cell Membranes using Zero-length Chemical Cross-linking and Mass Spectrometry (CX-MS)**; Roland Rivera-Santiago<sup>1,2</sup>; Sandra Harper<sup>2</sup>; Sira Sriswasdi<sup>3</sup>; David Speicher<sup>2</sup>;  
<sup>1</sup>University of Pennsylvania, Philadelphia, PA; <sup>2</sup>The Wistar Institute, Philadelphia, PA; <sup>3</sup>University of Tokyo, Tokyo, Japan
- WP 614 **Structural Proteomics Study of Native  $\alpha$ -synuclein in Solution**; Nicholas Brodie<sup>1</sup>; Evgeniy Petrotchenko<sup>1</sup>; Christoph Borchers<sup>1,2</sup>;  
<sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada; <sup>2</sup>Dept. of Biochem. & Microbiol., Univ. of Victoria, Victoria, BC, Canada
- WP 615 **Use of Ion Mobility and Cross Linking Mass Spectrometry with Hybrid Modelling to Delineate the Structure of CbpA**; Konstantinos Thalassinos<sup>1</sup>; Harpal Sahota<sup>1</sup>; Adam Cryar<sup>1</sup>; Maya Topf<sup>1</sup>;  
 Institute of Structural and Molecular Biology, London, UK
- WP 616 **Fragmentation and Aggregation of Physiological and Parkinson-Synucleins Revealed by Ion Mobility- MS and HDX- MS**; Michael Przybylski<sup>1</sup>; Kathrin Lindner<sup>1</sup>; Nicolas Pierson<sup>2</sup>; Ying Zhang<sup>3</sup>; Brindusa-Alina Petre<sup>1</sup>;

Stefan Schildknecht<sup>1</sup>; Michael Gross<sup>3</sup>; David Clemmer<sup>2</sup>;  
<sup>1</sup>Steinbeis Centre Biopolymer Analysis, Konstanz, Germany;  
<sup>2</sup>Indiana University Dept. Chemistry, Bloomington, IN;  
<sup>3</sup>Washington University St. Louis, St. Louis, MO

- WP 617 **HDL Particle Size Versus the HDL Proteome**; David Schieltz<sup>1</sup>; Jon Rees<sup>2</sup>; Zsuzsanna Kuklenyik<sup>1</sup>; Bryan Parks<sup>1</sup>; Michael Gardner<sup>1</sup>; Lisa McWilliams<sup>1</sup>; Yulanda Williamson<sup>1</sup>; John R Barr<sup>1</sup>;  
 Centers For Disease Control and Prevention, Atlanta, GA

### H/D EXCHANGE: PROTEIN STRUCTURE/FUNCTION I 618-647

- WP 618 **Discovering a Connection between Structural Sensitivity to pH & Interaction with FcRn in IgG1 Molecules**; Benjamin Walters<sup>1</sup>; Pernille F. Jensen<sup>3</sup>; Vincent Larraillet<sup>4</sup>; Tom Patapoff<sup>2</sup>; Kasper Rand<sup>3</sup>; Jennifer Zhang<sup>1</sup>;  
<sup>1</sup>Protein Analytical Chemistry, Genentech, South San Francisco, California; <sup>2</sup>Early Stage Pharmaceutical Development, Genentech, South San Francisco, California; <sup>3</sup>Dept. of Pharmacy, U. of Copenhagen, Copenhagen, Denmark; <sup>4</sup>pRed, Roche Innovation Center, Penzberg, Germany
- WP 619 **New Model for Prediction and Comparison of Per-residue Deuterium Uptake Level and Structure of Peptides Ion on the Gas Phase**; Samaneh Ghassabi Kondalaji<sup>1</sup>; Mahdiar Khakinejad<sup>1</sup>; Stephen Valentine<sup>2</sup>;  
<sup>1</sup>Morgantown, WV; <sup>2</sup>West Virginia University, Morgantown, WV
- WP 620 **HDX-MS Characterization of New Class of Multimerization Selective Inhibitors of HIV-1 Integrase**; Venkatasubramanian Dharmarajan<sup>1</sup>; Matthew Plumb<sup>2</sup>; Matthew Gibson<sup>2</sup>; Mamuka Kvaratskhelia<sup>2</sup>; Patrick R. Griffin<sup>1</sup>;  
<sup>1</sup>The Scripps Research Institute, Jupiter, FL; <sup>2</sup>The Ohio State University, Columbus, OH
- WP 621 **Effects of Class II and III UAB Rexinoids on the Dynamics of Nuclear Receptors by Hydrogen Deuterium Exchange Mass Spectrometry**; Amanda Proper<sup>1</sup>; Emily Cowart<sup>1</sup>; Donald Muccio<sup>1</sup>; Matthew Renfrow<sup>1</sup>;  
 University of Alabama at Birmingham, Birmingham, AL
- WP 622 **Examining Liposome Association and Small Molecule Inhibition of Fatty Acid Amide Hydrolase (FAAH) by Hydrogen/Deuterium Exchange Mass Spectrometry**; Brent Kochert<sup>1</sup>; Alexandros Makriyannis<sup>1</sup>; John Engen<sup>1</sup>;  
 Northeastern University, Boston, MA
- WP 623 **Characterization of the Conformation of Therapeutic Antibody Oxidation Variants with Optimized Hydrogen/Deuterium Exchange Mass Spectrometry**; Terry Zhang<sup>1</sup>; David Horn<sup>1</sup>; Shanhua Lin<sup>2</sup>; Xiaodong Liu<sup>2</sup>; Jonathan Josephs<sup>1</sup>;  
<sup>1</sup>ThermoFisher, San Jose, CA; <sup>2</sup>ThermoFisher, Sunnyvale, CA
- WP 624 **Assessment of HOS of IgG2 Monoclonal Antibodies using Two Proteases in a Single Column Approach to Enhance the Sequence Coverage**; Sasidhar N Nirudodhi<sup>1</sup>; Justin Sperry<sup>1</sup>; Jason Rouse<sup>2</sup>; James A. Carroll<sup>1</sup>;  
<sup>1</sup>Pfizer, Chesterfield, MO; <sup>2</sup>Pfizer, Inc., Andover, MA
- WP 625 **Hydrogen/Deuterium Exchange - Mass Spectrometry Reveals Conformational Changes between Human Phosphatase PP2C $\alpha$  and a Catalytically Inactive Metal Binding Site Mutant**; Elyssia S. Gallagher<sup>1,2</sup>; Subrata Debnath<sup>3</sup>; Sharlyn J. Mazur<sup>3</sup>; Lisa M. Miller Jenkins<sup>3</sup>; Stewart R. Durell<sup>3</sup>; Ettore Appella<sup>3</sup>; Jeffrey W. Hudgens<sup>1,2</sup>;  
<sup>1</sup>National Institute of Standards and Technology, Rockville, MD; <sup>2</sup>Institute for Bioscience & Biotechnology Research, Rockville, MD; <sup>3</sup>National Cancer Institute, NIH, Bethesda, MD
- WP 626 **Mapping Protein-Protein Interaction Sites and Protein Dynamics using HDXMS: How Binding to CK Stabilizes the Ankyrin Repeat Domain of ASB9**; Deepa Balasubramaniam<sup>1</sup>;  
 UCSD, La Jolla, CA

- WP 627 **Impact of Unpaired Cysteines on the Conformation and Antigen Binding of Two Different Monoclonal Antibodies by Hydrogen/Deuterium Exchange Mass Spectrometry;** Hui-Min Zhang; Jin Li; Ben Walters; Jennifer Zhang; Yung-Hsiang Kao; *Genentech, South San Francisco, CA*
- WP 628 **Stepwise Sequential Protein Folding by a Hydrogen Exchange – Mass Spectrometry Method;** Wenbing Hu; Zhongyuan Kan; Benjamin Walters; Leland Mayne; S. Walter Englander; *University of Pennsylvania, Philadelphia, PA*
- WP 629 **Hydrogen/deuterium Exchange Mass Spectrometry Reveals Soybean Lipoxygenase Conformational Flexibility;** Anthony T. Iavarone; Adam R. Offenbacher; Judith P. Klinman; *UC Berkeley, Berkeley, CA*
- WP 630 **Local Folding Energies/Rates of Wild-Type Staphylococcal Nuclease Determined by Protein Equilibrium Population Snapshot H/D Exchange Electrospray Ionization Mass Spectrometry (PEPS-HDX-ESI-MS);** Rohana Liyanage; Hayden Pacl; Julie Rhee; Jennifer Gidden; Wesley Stites; Jackson O Lay Jr; *University of Arkansas, Fayetteville, AR*
- WP 631 **Profiling Protein Dynamics in SET Domain Containing Proteins;** Kristian E. Teichert<sup>1,2</sup>; Roxana E. Iacob<sup>1</sup>; Thomas E. Wales<sup>1</sup>; Roodolph St. Pierre<sup>2</sup>; Mette Ishoey<sup>2</sup>; Sixun Chen<sup>3</sup>; Joshiawa Paulk<sup>2</sup>; James E. Bradner<sup>2</sup>; John R. Engen<sup>1</sup>; <sup>1</sup>*Northeastern University, Boston, MA*; <sup>2</sup>*Dana Farber Cancer Institute, Boston, MA*; <sup>3</sup>*Broad Institute, Cambridge, MA*
- WP 632 **Biophysical Analysis of the C-Terminal Tail of EGF Receptor Tyrosine Kinase using HDX-MS and Small-angle X-ray Scattering;** Theodore Keppel; Kwabena Sarpong; John Monsey; Jian Zhu; Ron Bose; *Washington University, St. Louis, MO*
- WP 633 **Probing the Interface between the Sulfite Reductase Subunits, Hemoprotein and Flavoprotein, by H/D Exchange monitored by FT-ICR MS;** Yeqing Tao<sup>1</sup>; Isabel Askenasy<sup>3</sup>; Nicolas L. Young<sup>2</sup>; M. Elizabeth Stroupe<sup>3</sup>; Alan G. Marshall<sup>1,2</sup>; <sup>1</sup>*Department of Chemistry and Biochemistry, Tallahassee, FL*; <sup>2</sup>*NHMFLL, Tallahassee, FL*; <sup>3</sup>*Department of Biological Science and Institute, Tallahassee, FL*
- WP 634 **Hydrogen Exchange Mass Spectrometry (HDX-MS) Reveals Local Structural Perturbations in Mutant Forms of Apolipoprotein A-I;** Christopher Wilson<sup>1</sup>; Madhurima Das<sup>2</sup>; Xiaohu Mei<sup>2</sup>; Olga Gursky<sup>2</sup>; John R. Engen<sup>1</sup>; <sup>1</sup>*Northeastern University, Boston, MA*; <sup>2</sup>*Boston University School of Medicine, Boston, MA*
- WP 635 **Investigation of Protein-Protein Interactions in the Human Pyruvate Dehydrogenase Complex by Hydrogen/Deuterium Exchange Mass Spectrometry;** Junjie Wang<sup>1</sup>; Jieyu Zhou<sup>1</sup>; Natalia S. Nemeria<sup>1</sup>; Mulchand S. Patel<sup>2</sup>; Frank Jordan<sup>1</sup>; <sup>1</sup>*Rutgers, the State University of New Jersey, Newark, NJ*; <sup>2</sup>*University at Buffalo, Buffalo, NY*
- WP 636 **Unraveling Dynamic Interactions within the Peripheral Stalk of F<sub>1</sub>F<sub>0</sub> ATP Synthase by HDX-MS;** Courtney Fast; Siavash Vahidi; Carla Busnello; Yumin Bi; Stanley Dunn; Lars Konermann; *Univ. of Western Ontario, London, ON*
- WP 637 **A Key Tryptophan in the Tec-family Tyrosine Kinase Btk Allosterically Regulates Kinase Activation;** Thomas E. Wales<sup>1</sup>; Raji E. Joseph<sup>2</sup>; Amy H. Andreotti<sup>2</sup>; Amy H. Andreotti<sup>2</sup>; John R. Engen<sup>1</sup>; <sup>1</sup>*Northeastern University, Boston, MA*; <sup>2</sup>*Iowa State University, Ames, IA*
- WP 638 **How Well Do We Understand Protein HDX Protection Patterns? A Molecular Dynamics Simulation Study;** Robert McAllister; Lars Konermann; *Univ. of Western Ontario, London, ON*
- WP 639 **Ligand-Induced Changes in Structure and Dynamics of the Dihydrodipicolinate (DHDPS) Synthase Enzyme Complex Studied by HDX-MS;** Modupeola Sowole<sup>1</sup>; Sarah Simpson<sup>2</sup>; Yulia Skovpen<sup>2</sup>; David Palmer<sup>2</sup>; Lars Konermann<sup>1</sup>; <sup>1</sup>*University of Western Ontario, London, Canada*; <sup>2</sup>*University of Saskatchewan, Saskatoon, Canada*
- WP 640 **Structural Analysis of SynGAP by HDX-MS;** Quinlin Hanson; Eric Underbakke; *Iowa State University, Ames, IA*
- WP 641 **Combining Native MS, IM-MS and HDX-MS for Structural Characterization of Bcd1p/Rtt106p complex involved in the box C/D snoRNPs Assembly Machinery;** Guillaume Terral<sup>1</sup>; Benoit Bragantini<sup>2</sup>; Jean-Michel Saliou<sup>1</sup>; Alain Van Dorsselaer<sup>1</sup>; Xavier Manival<sup>2</sup>; Bruno Charpentier<sup>2</sup>; Sarah Cianféroni<sup>1</sup>; <sup>1</sup>*Laboratoire de Spectrométrie de Masse BioOrganique, Strasbourg, France*; <sup>2</sup>*Ing. Moléculaire et Physiopathologie Articulaire, Vandoeuvre-lès-Nancy, France*
- WP 642 **Gas-phase Hydrogen/Deuterium Exchange can be Used to Detect Conformational Differences in Protein Structure and Distinguish between Conformational Families;** Helen S Beeston<sup>1</sup>; James R Ault<sup>1</sup>; Henry C Fisher<sup>1</sup>; Steven D Pringle<sup>2</sup>; Jeffrey M Brown<sup>2</sup>; Alison E Ashcroft<sup>1</sup>; <sup>1</sup>*University of Leeds, Leeds, UK*; <sup>2</sup>*Waters Corporation, Wilmslow, UK*
- WP 643 **Protein Structural Dynamics at the Gas/Water Interface Examined by Hydrogen Exchange Mass Spectrometry;** Yiming Xiao<sup>1</sup>; Lars Konermann<sup>2</sup>; <sup>1</sup>*University of Western Ontario, London, Canada*; <sup>2</sup>*Univ. of Western Ontario, London, ON*
- WP 644 **Lipid Packing Density Alters the Conformation of Membrane-Associated HIV-1 Nef;** Gregory F. Pirrone<sup>1</sup>; Michael S. Kent<sup>2</sup>; John R. Engen<sup>1</sup>; <sup>1</sup>*Northeastern University, Boston, MA*; <sup>2</sup>*Sandia National Laboratories, Albuquerque, NM*
- WP 645 **Tryptophan289 Single Point Mutation Modulates the Dynamic Properties of Human Monoacylglycerol Lipase: A Hydrogen Deuterium Exchange Mass Spectrometry Study;** Ioannis Karageorgos<sup>1,2</sup>; Elyssia S. Gallagher<sup>1,2</sup>; Nikolai Zvonok<sup>3</sup>; Alexandros Makriyannis<sup>3</sup>; Jeffrey W. Hudgens<sup>1,2</sup>; <sup>1</sup>*National Institute of Standards and Technology, Rockville, MD*; <sup>2</sup>*Institute for Bioscience & Biotechnology Research, Rockville, MD*; <sup>3</sup>*Center for Drug Discovery, Northeastern University, Boston, MA*
- WP 646 **Millisecond HX-MS to Detect Residual Helicity in a Disordered Protein using a Denatured State Reference;** Mohammed Al-Naqshabandi<sup>1,2</sup>; David D. Weis<sup>1</sup>; <sup>1</sup>*University of Kansas, Lawrence, ks*; <sup>2</sup>*Soran University, Erbil, Iraq*

**PROTEINS: CONFORMATION ANALYSIS**  
648-658

- WP 648 **Influence of Lipid Environment on Gramicidin A Dimer Conformation Probed using Nanodiscs and ESI-IMS-MS;** Emma-Dune Leriche; Xuxin Fan; Elena N. Kitova; John S. Klassen; *University of Alberta, Edmonton, Canada*
- WP 649 **Conformational Changes of an Allosteric Enzyme Probed in Solution and in the Gas-Phase: IM-MS, HDX-MS and AUC Studies of MtATP-phosphoribosyltransferase;** Kamila Pacholarz<sup>1,2</sup>; Thomas Jowitt<sup>1</sup>; Rebecca Burnley<sup>3</sup>; Victoria Ordsmith<sup>2</sup>; Massimiliano Porrini<sup>4</sup>; Gérald Larrouy-Maumus<sup>5</sup>; João Pisco<sup>5</sup>; Rachel Garlish<sup>3</sup>; Richard Taylor<sup>3</sup>; Luiz de Carvalho<sup>5</sup>; Perdita Barran<sup>1</sup>; <sup>1</sup>*University of Manchester, Manchester, UK*; <sup>2</sup>*University of Edinburgh, Edinburgh, UK*; <sup>3</sup>*UCB, Slough, UK*; <sup>4</sup>*Institute Européen de Chimie et Biologie, Pessac, France*; <sup>5</sup>*MRC National Institute for Medical Research, London, UK*
- WP 650 **Probing GPCR-ligand Interaction by Chemical Crosslinking and Mass Spectrometry;** Bill Huang; Ji-Won Lee; Hee-Yong Kim; *NIAAA/NIH, Rockville, MD*
- WP 651 **Insights into Gas-phase Protein Conformations from Matrix Assisted Ionization (MAI) using Ion Mobility Spectrometry-Mass Spectrometry;** Daniel Woodall<sup>1</sup>; Shameemah Thawoos<sup>1</sup>; Corinne Lutomski<sup>1</sup>; Sarah Trimpin<sup>1,2</sup>; <sup>1</sup>*Wayne State University, Detroit, MI*; <sup>2</sup>*Cardiovascular Research Institute, Detroit, MI*



- WP 652 **Development of a Rapid & Sensitive Shape Selective Screen to Monitor the Folding/Assembly of Recombinant Proteins;** Owen Cornwell<sup>1</sup>; Daniel Higazi<sup>2</sup>; Nicholas Bond<sup>2</sup>; Matthew Edgeworth<sup>1</sup>; James Scrivens<sup>1</sup>; <sup>1</sup>University of Warwick, Coventry, UK; <sup>2</sup>MedImmune, Cambridge, UK
- WP 653 **Ion Mobility Mass Spectrometry Reveals (Non)-Structural Order in p27;** Rebecca Beveridge<sup>1</sup>; Yongqi Huang<sup>2</sup>; Rahul Das<sup>3</sup>; Rohit Pappu<sup>3</sup>; Richard Kriwacki<sup>2</sup>; Perdita Barran<sup>1</sup>; <sup>1</sup>University of Manchester, Manchester, UK; <sup>2</sup>St. Jude Children's Research Hospital, Memphis, TN; <sup>3</sup>Washington University, St. Louis, MO
- WP 654 **Protein Conformational Study by Selected Accumulation Ion Mobility Spectrometry-Electron Capture Dissociation Tandem Mass Spectrometry;** Yi Pu<sup>1</sup>; Rebecca S. Glaskin<sup>2</sup>; Mark E. Ridgeway<sup>3</sup>; Melvin A. Park<sup>3</sup>; Cheng Lin<sup>2</sup>; Catherine E. Costello<sup>1,2</sup>; <sup>1</sup>Boston University, Boston, MA; <sup>2</sup>Boston University School of Medicine, Boston, MA; <sup>3</sup>Bruker Daltonics, Billerica, MA
- WP 655 **Effect of Post-Translational Modifications on the Metal Binding and Conformation of Alpha-Synuclein;** Aimee Paskins; Rebecca Mason; Cathrine Duckett; Caroline Dalton; David Smith; *Sheffield Hallam University, Sheffield, UK*
- WP 656 **Analysis of p85 $\alpha$  Molecular Architecture using Chemical Cross-Linking;** Evan T Brower<sup>1</sup>; Raghothama Chaerkady<sup>1</sup>; Qing Wang<sup>1</sup>; Mathias Schäfer<sup>2</sup>; Andrea Sinz<sup>3</sup>; Kenneth W. Kinzler<sup>1</sup>; Bert Vogelstein<sup>1</sup>; L. Mario Amzel<sup>1</sup>; Robert N. Cole<sup>1</sup>; Sandra B. Gabelli<sup>1</sup>; <sup>1</sup>Johns Hopkins University, Baltimore, MD; <sup>2</sup>Universität zu Köln, Greinstrasse, Germany; <sup>3</sup>Martin-Luther-Universität, Halle-Wittenberg, Germany
- WP 657 **Twisting the Twist: an Ion Mobility-Mass Spectrometry study of the p53:MDM2 interaction;** Eleanor Dickinson; *University of Manchester, Manchester, UK*
- WP 658 **Mapping the Protein Structural Changes by Quantitative Cross-linking;** Zdenek Kukacka<sup>1,2</sup>; Michal Rosulek<sup>1,2</sup>; Daniel Kavan<sup>1,2</sup>; Petr Pompach<sup>1,2</sup>; Petr Novak<sup>1,2</sup>; <sup>1</sup>Institute of Microbiology, Prague, Czech Republic; <sup>2</sup>Charles University, Prague, Czech Republic
- ANTIBODIES AND ANTIBODY: DRUG CONJUGATES I**  
**659-687**
- WP 659 **Characterization of Host Cell Proteins in the Protein A Purification of a Variety of Monoclonal Antibodies;** Chong-Feng Xu; Zhenzhen Wang; Daniel Xu; Christina Alves; Li Zang; *Biogen Idec, Cambridge, MA*
- WP 660 **Mass Spectrometry Characterization of SJCD3 MAb and Comparison with OKT3;** Bo Zhai<sup>1</sup>; Aaron Shafer<sup>1</sup>; Kevin van Cott<sup>2</sup>; Chao-Xuan Zhang<sup>1</sup>; Michael Meagher<sup>1</sup>; <sup>1</sup>St Jude Children's Research Hospital, Memphis, TN; <sup>2</sup>University of Nebraska-Lincoln, Lincoln, NE
- WP 661 **A Universal Solution for the Pre-Clinical Bioanalysis of Humanized Therapeutic Monoclonal Antibodies in Plasma;** Kwasi Antwi; Urban Kieman; Eric Niederkofler; *Thermo Fisher Scientific, Tempe, AZ*
- WP 662 **In-depth Identification of Protein Images by Combining High Mass Resolution MALDI-FTICR Imaging and High Performance qTOF nLC-MS/MS;** Arnd Ingendoh<sup>1</sup>; Matt Willetts<sup>2</sup>; Shannon Cornett<sup>2</sup>; <sup>1</sup>Bruker Daltonik, Bremen, Germany; <sup>2</sup>Bruker Daltonics, Billerica, MA
- WP 663 **Comprehensive Characterization of a Representative Antibody-Drug Conjugate by CESI-MS;** Bryan Fonslow<sup>2</sup>; Eric Johansen<sup>1</sup>; Hans Dewald<sup>2</sup>; <sup>1</sup>SCIEX, Redwood City, CA; <sup>2</sup>SCIEX, Brea, CA
- WP 664 **Rapid Identification and Quantitation of Disulfide Bonds in Antibodies and Other Purified Proteins;** Wilfred H. Tang; Yong Joo Kil; Kevin L. Crowell; Marshall W. Bern; Eric Carlson; Chris Becker; *Protein Metrics Inc., San Carlos, CA*
- WP 665 **Characterization of Monoclonal Antibodies and ADCs using a Benchtop Orbitrap Mass Spectrometer;** Xiaoxi Zhang; *ThermoFisher Scientific, Shanghai, China*
- WP 666 **Exact de novo Sequencing of a Monoclonal Antibody with Fab Glycosylation;** Marshall W. Bern<sup>1</sup>; David Morgenstern<sup>2</sup>; Beatrix Ueberheide<sup>2</sup>; Walter Bogdanoff<sup>3</sup>; Rebecca Dubois<sup>3</sup>; <sup>1</sup>Protein Metrics, San Carlos, CA; <sup>2</sup>New York University, New York, NY; <sup>3</sup>University of California, Santa Cruz, CA
- WP 667 **De novo Sequencing Our Polyclonal Immune Response Without B-cell Sequencing;** Adrian Guthals<sup>1</sup>; Yutian Gan<sup>2</sup>; Wendy Sandoval<sup>2</sup>; Nuno Bandeira<sup>1,3</sup>; <sup>1</sup>University of California, San Diego, La Jolla, CA; <sup>2</sup>Genentech, South San Francisco, CA; <sup>3</sup>Skaggs School of Pharmacy, UC San Diego, La Jolla, CA
- WP 668 **Investigation of Anti-Drug-Antibody Impact on LC-MS/MS Bioanalysis of Unconjugated Payload of Antibody Drug Conjugate in a Monkey Toxicity Study;** Hang Zeng<sup>1</sup>; Ragu Ramanathan<sup>1</sup>; Frank Barletta<sup>1</sup>; Michael Giovannelli<sup>2</sup>; Rick Steenwyk<sup>1</sup>; <sup>1</sup>PDM, Pfizer, Inc., Groton, CT; <sup>2</sup>DSRD, Pfizer, Inc, Groton, CT
- WP 669 **Understanding of Critical Quality Attributes of Biopharmaceuticals In Vivo;** Yinyin Li<sup>1</sup>; Emma Zhang<sup>2</sup>; Peter Li<sup>2</sup>; Billy Wu<sup>2</sup>; Patrick Swann<sup>1</sup>; Yelena Lyubarskaya<sup>1</sup>; <sup>1</sup>Biogen Idec, Cambridge, MA; <sup>2</sup>BioAnalytix Inc, Cambridge, MA
- WP 670 **Characterization of Degradants of a Therapeutic Monoclonal Antibody via Combined Topdown and Bottom Up LC-MS/MS;** Antonio Triolo<sup>1</sup>; Elisa Libralesso<sup>1</sup>; Francesca Boscaro<sup>2</sup>; Francesca Romana Dani<sup>2</sup>; Elena Michelucci<sup>2</sup>; Giuseppe Pieraccini<sup>2</sup>; Gloriano Moneti<sup>2</sup>; <sup>1</sup>Menarini Ricerche Spa, Firenze, Italy; <sup>2</sup>CISM Centro di Servizi di Spettrometria di Massa, Firenze, Italy
- WP 671 **Localizing the Conjugation Sites of Cysteine-Conjugated Antibody Drug Conjugates by Improved LC-MS Subunit Analysis for ADC Positional Isomer Identification;** Henry Shion<sup>1</sup>; Robert Birdsall<sup>1</sup>; Liuxi Chen<sup>1</sup>; Ying-Qing Yu<sup>1</sup>; Frank W. Kotch<sup>3</sup>; April Xu<sup>2</sup>; Thomas J. Porter<sup>4</sup>; Weibin Chen<sup>1</sup>; <sup>1</sup>Waters Biopharmaceutical Business Operations, Milford, MA; <sup>2</sup>Pfizer Analytical Research & Development, Pearl River, NY; <sup>3</sup>Pfizer Bioprocess Research & Development, Pearl River, NY; <sup>4</sup>Pfizer Analytical Research & Development, Andover, MA
- WP 672 **Rapid LC/MS Identification of mAbs Utilizing CDR Masking;** Amy Hilderbrand<sup>1</sup>; Rashmi Jain<sup>2</sup>; Nisana Andersen<sup>1</sup>; Benjamin Moore<sup>1</sup>; Chenchen Wang<sup>1</sup>; Cleo Salisbury<sup>1</sup>; <sup>1</sup>Genentech, South San Francisco, CA; <sup>2</sup>University of California San Diego, San Diego, CA
- WP 673 **Evaluation of Hemoglobin as a Carrier of Anti-HIV Drug (Adefovir) in Macrophage-targeting Drug Delivery System;** Shengsheng Xu; Igor A. Kaltashov; *University of Massachusetts-Amherst, Amherst, Massachusetts*
- WP 674 **Analysis of Antibody Drug Conjugate using High Flow HPLC Coupled to Time-of-Flight Mass Spectrometry;** Ravindra Gudihal; Sundaram M Palaniswamy; Sudha Rajagopalan; *Agilent Technologies India Pvt. Ltd, Bangalore, India*
- WP 675 **Immunocapture LC-MS/MS Hybrid Assays for Conjugated-Antibody and Total-Antibody in Antibody Drug Conjugate (ADC) Bioanalysis;** Huidong Gu; Ang Liu; Frank Zambito; Alexander Kozhich; Heather Myler; Anne-Françoise Aubry; Mark Arnold; Jian Wang; *Bristol-Myers Squibb, Princeton, NJ*
- WP 676 **Full Validation of Therapeutic Antibody Sequences by Middle-Up Mass Measurements and Middle-Down Protein Sequencing;** Anja Resemann<sup>1</sup>; Wolfgang Jabs<sup>1</sup>; Anja Wiechmann<sup>1</sup>; Elsa Wagner<sup>2</sup>; Olivier Colas<sup>2</sup>; Waltraud Evers<sup>1</sup>; Eckhard Belau<sup>1</sup>; Lars Vorweg<sup>1</sup>; Catherine Evans<sup>3</sup>; Alain Beck<sup>2</sup>; Detlev Suckau<sup>1</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup>Centre d'Immunologie Pierre-Fabre,



## WEDNESDAY POSTERS

St. Julien-en-Genevois, France; <sup>3</sup>Bruker Daltonics Ltd, Coventry, UK

WP 677 **Enhancing Characterization Antibody-based Biologic using Differential Mobility and Mass Spectrometry;** Tanya Gamble<sup>1</sup>; J.C. Yves Leblanc<sup>1</sup>; Eric Johansen<sup>2</sup>; Suma Ramagiri<sup>1</sup>; <sup>1</sup>SCIEX, Concord, ON, ON; <sup>2</sup>SCIEX, Redwood, CA

WP 678 **Comprehensive LC/MS Characterization of a Broadly Neutralizing HIV-1 mAb;** Li Cao; Vera Ivleva; Jie Liu; Deepika Gollapudi; Jonathan Cooper; Richard Schwartz; VPP, NIAID, NIH, Gaithersburg, MD

WP 679 **Application of Data Independent Acquisition for Top-Down Characterization of IgG Light;** Sahana Mollah; Melanie Juba; Xu Wang; AB SCIEX, Redwood City, CA

WP 680 **Mass Spectrometry Rearrangement by Collision Induced Dissociation of Cleavable ADC Linker Containing Aminobenzylcarbamate Group;** Xidong Feng; Dahui Zhou; Kenneth Dirico; Russell G Dushin; Chakrapani Subramanyam; Christopher J O'Donnell; Justin Stroh; Michael J Shapiro; Pfizer Worldwide Research, Groton, CT

WP 681 **Characterization of Glycosylation and Amino Acid Sequence Features of Pig Immunoglobulins;** Paul Lopez<sup>1</sup>; Lauren Girard<sup>1</sup>; Andrey Oliveira<sup>1</sup>; Edward Bodnar<sup>1</sup>; Apolline Salama<sup>2</sup>; Jean-Paul Soullou<sup>2</sup>; Helene Perreault<sup>1</sup>; <sup>1</sup>University of Manitoba, Winnipeg, Canada; <sup>2</sup>UMR INSERM 10-64, Université de Nantes, Nantes, France

WP 682 **A Universal Immunocapture-LC-MS/MS Workflow for Biological Compound Quantitation in Preclinical Studies;** Lei Xiong<sup>1</sup>; Witold Woroniecki<sup>1</sup>; Suma Ramagiri<sup>2</sup>; Gary Impey<sup>2</sup>; Hua-Fen Liu<sup>1</sup>; <sup>1</sup>AB SCIEX, Redwood City, California; <sup>2</sup>AB SCIEX, Concord, ON

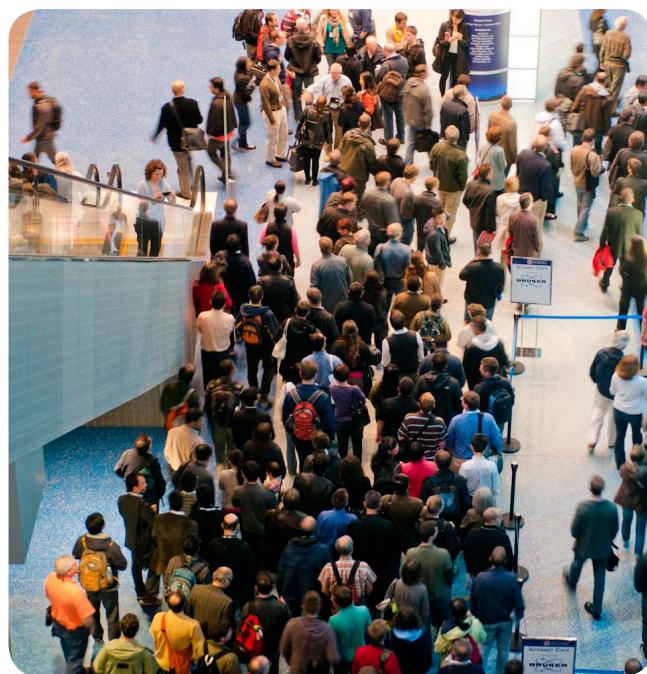
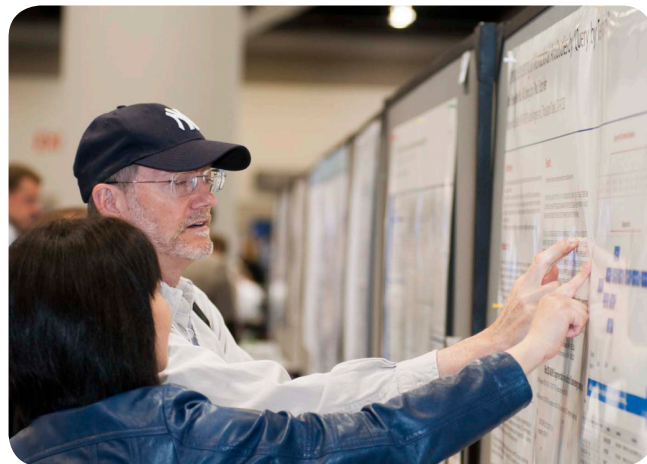
WP 683 **Characterization of Charge Variants of Therapeutic Antibodies A (taA) in CEX Fractions by Bottom-up and Top-down MS;** Chien-Wen Hung; Benedetto Aquilino; Urs Hanke; Claudia Torella; Christoph Roesli; Florian Wolschin; Andreas Seidl; Sandoz Biopharmaceuticals, Oberhaching, Germany

WP 684 **Two Approaches that Facilitate Antibody Analysis;** Nick DeGraan-Weber; James P. Reilly; Indiana University, Bloomington, IN

WP 685 **Automated Affinity Capture and Rapid On-Tip Digestion to Accurately Quantitate in vivo Deamidation of Therapeutic Antibodies;** John C. Tran; Daniel Tran; Phillip Chu; Denise Krawitz; Amy Hilderbrand; Kathy Kozak; Yichin Liu; Jianyong Wang; Genentech, South San Francisco, CA

WP 686 **Rapid Comprehensive Comparison of Five Versions of Bevacizumab – Avastin versus Its Biosimilars;** Chris Becker<sup>1</sup>; Yong Kil<sup>1</sup>; Eric Carlson<sup>1</sup>; David Morgenstern<sup>2</sup>; Beatrix Ueberheide<sup>2</sup>; <sup>1</sup>Protein Metrics Inc., San Carlos, CA; <sup>2</sup>NYU School of Medicine, New York, NY

WP 687 **Top Down LC/MS Characterization of RP-HPLC Impurities of Monoclonal Antibody by High Energy Collision –Induced Dissociation;** Jia Zhao; flora gu; yan-hui liu; Huijuan Li; Mohammed shameem; Merck, Kenilworth, NJ





7:30 – 8:00 am..... Set up all Thursday posters  
 10:30 am – 1:00 pm..... Odd-numbered posters present  
 12:00 – 2:30 pm..... Even-numbered posters present  
 2:30 pm..... Remove all Thursday posters

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Ion Mobility: Small Molecule and Metabolomics.....	640-652
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Imaging MS: Small Molecules.....	672-689

#### AMBIENT IONIZATION: FUNDAMENTALS 001-019

- ThP 001 **Effect of Humidity on Ionization Efficiencies in Dopant-Assisted GC-APCI-TOF MS;** Carolyn Hutchinson; Daniel Cole; Young Jin Lee; *Iowa State University, Ames, IA*
- ThP 002 **High Sensitive and Throughput Direct Analysis of Genotoxicity Acrylamide Generated by High Temperature Food Processes using DART-MS Combined with Corona++™;** Motoshi Sakakura<sup>1</sup>; Hiroshi Hike<sup>1</sup>; Takatomo Kawamukai<sup>1</sup>; Teruhisa Shiota<sup>1</sup>; Kanako Sekimoto<sup>2</sup>; Mitsuo Takayama<sup>2</sup>; <sup>1</sup>AMR Inc., Meguro-Ku, Japan; <sup>2</sup>Yokohama City Univ., Yokohama, Japan
- ThP 003 **Comparison of Internal Energy Distributions of Ions Created by Electrospray Ionization and Laser Ablation-Liquid Vortex Capture/Electrospray Ionization;** John F. Cahill; Vilmos Kertesz; Olga S. Ovchinnikova; Gary J. Van Berkel; *Oak Ridge National Laboratory, Oak Ridge, TN*
- ThP 004 **Particle Size Measurement from Tissue Ablation for Laser Ambient Ionization and Sampling;** Fan Cao; Kermit K. Murray; *Louisiana State University, Baton Rouge, LA*
- ThP 005 **The Potential of Peptide/Protein Arrays using Desorption Electrospray Ionisation Mass Spectrometry; Sensitivity and Limit of Detection;** Elzbieta Gurdak<sup>1</sup>; Andrew Hook<sup>2</sup>; Alexander Shard<sup>1</sup>; Josephine Bunch<sup>1</sup>; <sup>1</sup>National Physical Laboratory, Teddington, UK; <sup>2</sup>University of Nottingham, Nottingham, UK
- ThP 006 **Comparison of Negative Ion ESI Ionization Efficiencies for a Diversity of Small Acidic Molecules with Widely Varying pK<sub>a</sub>'s;** James Mattila; Shelsea Hurdle; Stephen Lucas; Christine A. Hughey; *James Madison University, Harrisonburg, VA*
- ThP 007 **Extractive Electrospray Ionization Mass Spectrometry with Metal Cationization;** Kenneth Swanson; Sandra Spencer; Gary L. Glish; *Univ. of North Carolina at Chapel Hill, Chapel Hill, NC*
- ThP 008 **Corona Discharge Suppression in Negative-ion Mode Nanoelectrospray via Trifluoroethanol Addition;** Phillip McClory; Kristina Hakansson; *University of Michigan, Ann Arbor, MI*
- ThP 009 **Collision Surfaces and Ambient Ionization Mechanisms; Studies Leading to the Improvement of Signal Intensities in Rapid Evaporative Ionization Mass Spectrometry;** Emrys A Jones<sup>1</sup>; Ottmar Golf<sup>1</sup>; Steven Pringle<sup>2</sup>; Tamas Karancsi<sup>3</sup>; Zoltan Takats<sup>1</sup>; <sup>1</sup>Imperial College London, London, UK; <sup>2</sup>Waters Corporation, Manchester, UK; <sup>3</sup>Waters Research Center, Budapest, Hungary

- ThP 010 **Benzyl Carbanion Transfer in the Fragmentation of N-(phenylsulfonyl)-benzeneacetamides: A Gas-phase Intramolecular SNAr Reaction;** Shanshan Shen; Yunfeng Chai; Yaqin Liu; Chang Li; Yuanjiang Pan; *Zhejiang University, Hangzhou, China*
- ThP 011 **A Study of the Gas-Phase Chemistry in a Dielectric Barrier Discharge using Argon and Hydrogen-Doped Argon as the Support Gases;** Wade Ellis; Paul Farnsworth; *Brigham Young University, Provo, UT*
- ThP 012 **Contained-Electrospray: A New Spray Ionization Process for Improving Ion Yields for Complex Samples during ESI-MS Analysis;** Dmytro Kulyk; Abraham Badu Tawiah; *Ohio State University, Columbus, OH*
- ThP 013 **Zero Volt Paper Spray Ionization and its Mechanism;** Yafeng Li<sup>1</sup>; Michael Wlekinski<sup>1</sup>; Soumabha Bag<sup>1</sup>; Depanjan Sarkar<sup>2</sup>; Rahul Narayanan, T. Pradeep<sup>2</sup>; R. Graham Cooks<sup>1,2</sup>; <sup>1</sup>Purdue University, West Lafayette, Indiana; <sup>2</sup>Indian Institute of Technology Madras, Chennai, India
- ThP 014 **Generation of Multiply Charged Ions using a liquid AP MALDI Ion Source without Heated Ion Transfer Tube;** Pavel Ryumin<sup>1</sup>; Jeff Brown<sup>1,2</sup>; Rainer Cramer<sup>1</sup>; <sup>1</sup>University of Reading, Reading, UK; <sup>2</sup>Waters Corporation, Wilmslow, UK
- ThP 015 **A Comparison of Atmospheric Pressure Surface Sampling Methods: DESI, PADI, AP-MALDI and LESA;** Tara La Roche Salter<sup>1</sup>; Rory Steven<sup>1</sup>; Elizabeth Randall<sup>1,2</sup>; Alan Race<sup>1</sup>; Ian Gilmore<sup>1</sup>; Josephine Bunch<sup>1,3</sup>; <sup>1</sup>National Physical Laboratory, Teddington, UK; <sup>2</sup>University of Birmingham, Birmingham, UK; <sup>3</sup>University of Nottingham, Nottingham, UK
- ThP 016 **Hydrophobic Paper Spray Ionization Mass Spectrometry;** Kathryn M. Davis; Abraham Badu-Tawiah; *The Ohio State University, Columbus, OH*
- ThP 017 **Surface-modified Wooden-tip Electrospray Ionization Mass Spectrometry for Enhanced Detection of Analytes in Complex Samples: Mechanism and Applications;** Bin Hu<sup>1</sup>; Yun-Yun Yang<sup>2</sup>; Jie-Wei Deng<sup>1,3</sup>; Zhong-Ping Yao<sup>1</sup>; <sup>1</sup>Hong Kong Polytechnic University, Hong Kong, China; <sup>2</sup>China National Analytical Center Guangzhou, Guangzhou, China; <sup>3</sup>Sun Yat-Sen University, Guangzhou, China
- ThP 018 **Fundamental Studies of Atmospheric Pressure Dielectric Barrier Discharge Jet used for Depth Profiling Mass Spectrometry;** Gerardo Gamez; Songyue Shi; Xiaoxia Gong; Marcel Kroschok; John Usala; *Texas Tech University, Lubbock, TX*
- ThP 019 **Toward Understanding Factors that Influence Globular Protein Ion Charge in Native Electrospray Ionization;** Anna Susa; Evan Williams; *Berkeley, CA*

**INSTRUMENTATION: MINI/PORTABLE/FIELDABLE MS  
020-032**

- ThP 020 **Development, Study and Application of Hand Portable GC/MS as a Field Investigative Tool for the First Responder**; Gareth Dobson; *Smiths Detection, Edgewood, MD*
- ThP 021 **The Research of the Scan Function About Linear Ion Trap at Low Vacuum**; Hao Lv<sup>1</sup>; Zhanfeng Zhao<sup>1</sup>; Eric Handberg<sup>2</sup>; Zhiquan Zhou<sup>1</sup>; <sup>1</sup>*Harbin Institute of Technology at Weihai, Weihai, China*; <sup>2</sup>*East China Institute of Tech., Nanchang, China*
- ThP 022 **Application of Sub-Ambient Pressure Gas Chromatography to the Development of a Miniature Ion-Trap GC/MS**; Conor Mullens; Daniel Debord; Corey Stedwell; Michael Spencer; David Rafferty; *1st Detect, Webster, TX*
- ThP 023 **Improvements to Membrane Inlet Interface for Subsea *in-situ* mass spectrometry**; Brian Gregson; Gary Hendrick; David Fries; *Spyglass Technologies, Inc., St. Petersburg, FL*
- ThP 024 **Evaluating Ion Trap Materials for Hand Portable, High Pressure Mass Spectrometry**; Kenion Blakeman; Tina Stacy; Craig Cavanaugh; J. Michael Ramsey; *University of North Carolina, Chapel Hill, NC*
- ThP 025 **Combining Real-Time Portable Membrane Introduction Mass Spectrometer and Whole Air Sampling Canister Data for Atmospheric Analysis of Volatile Organic Compounds**; Nicholas G. Davey<sup>1,4</sup>; Ryan J. Bell<sup>3,4</sup>; Isobel J. Simpson<sup>2</sup>; Donald R. Blake<sup>2</sup>; Erik T. Krogh<sup>1,4</sup>; Christopher G. Gill<sup>1,4</sup>; <sup>1</sup>*University of Victoria, Victoria, BC, Canada*; <sup>2</sup>*UC Irvine, Irvine, CA*; <sup>3</sup>*Beaver Creek Analytical LLC, Boulder, CO*; <sup>4</sup>*Appl. Env. Res. Labs. (AERL), Nanaimo, Canada*
- ThP 026 **Optimization of the Cylindrical Ion Trap Geometry Operated at High Pressure**; Dmitriy Chernookiy; Bruno Coupier; J. Michael Ramsey; *University of North Carolina, Chapel Hill, Chapel Hill, NC*
- ThP 027 **Low Voltage RF Amplitude Scanning with Multi-Frequencies for Ion Trap Mass Spectrometry**; Seung Yong Kim<sup>1</sup>; Jong Rok Ahn<sup>1</sup>; Wanseop Jeong<sup>1</sup>; Mo Yang<sup>1</sup>; Eunnam Kim<sup>2</sup>; Jin-Young Choi<sup>2</sup>; Hyun Sik Kim<sup>1</sup>; <sup>1</sup>*Korea Basic Science Institute, Ochang-Eup Cheongju-Si, South Korea*; <sup>2</sup>*Korea University, Seoul, Korea*
- ThP 028 **Real-time Sample Analysis using Remote Sampling Probe and Miniature Mass Spectrometer**; Chien-Hsun Chen<sup>1</sup>; Ziqing Lin<sup>1</sup>; R. Graham Cooks<sup>2</sup>; Zheng Ouyang<sup>1</sup>; <sup>1</sup>*Biomedical Engineering, Purdue University, West Lafayette, IN*; <sup>2</sup>*Chemistry Department, Purdue University, West Lafayette, IN*
- ThP 029 **Manipulation of Trapped Ions in High Pressures in CITs and SLITs**; Andrew Hampton; J. Michael Ramsey; *UNC - Chapel Hill, Chapel Hill, NC*
- ThP 030 **Making Sense of Water Quality: A Portable MS-UV Sensing Platform for Real-Time Monitoring in Aquaculture**; Simon Maher<sup>1,3</sup>; Barry Smith<sup>2</sup>; Mariya Juno<sup>3</sup>; Fred Jjunju<sup>3</sup>; Behnam Bastani<sup>1,3</sup>; Lei Su<sup>3</sup>; Urszula Salaj-Kosla<sup>4</sup>; Liam Lewis<sup>4</sup>; Jean-Michel Mortz<sup>5</sup>; Dag Hammer<sup>6</sup>; Gyda Christophersen<sup>6</sup>; Pat O'Leary<sup>7</sup>; Allan MacMaster<sup>8</sup>; Stephen Taylor<sup>2,3</sup>; Iain Young<sup>1</sup>; <sup>1</sup>*Institute of Integrative Biology, University of Liverpool, UK*; <sup>2</sup>*Q Technologies, Liverpool, UK*; <sup>3</sup>*Dept. Electrical Engineering & Electronics, University of Liverpool, UK*; <sup>4</sup>*Cork Institute of Technology, Cork, Ireland*; <sup>5</sup>*BAMO-IER GmbH, Mannheim, Germany*; <sup>6</sup>*Teknologisk Institutt as, Oslo, Norway*; <sup>7</sup>*Faaltch Technologies, Cork, Ireland*; <sup>8</sup>*Anglesey Aquaculture Ltd, Beaumaris, UK*
- ThP 031 **Characterization of Small Organic Molecules and Proteins by Matrix-Assisted Ionization-Portable Mass Spectrometry**; Zachary Devereaux; Sarah Trimpin; *Wayne State University, Detroit, MI*

- ThP 032 **Improvement of a Micro- Time of Flight Mass-Spectrometer based on MEMS Technologies**; Romain Mahieu<sup>2</sup>; Laurent Duraffourg<sup>2</sup>; Marc Gely<sup>2</sup>; Thomas Alava<sup>2</sup>; Charles-Marie Tasseti<sup>1</sup>; Frederic Progent<sup>1</sup>; <sup>1</sup>*CEA, DAM, DIF, F-91297 Arpajon, France*; <sup>2</sup>*CEA LETI, Grenoble, France*

**GCMS: INSTRUMENTATION AND APPLICATIONS  
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- ThP 033 **Analysis of FAMES Using Cold EI GC/MS for Enhanced Molecular Ion Selectivity**; Adam J. Patkin; Sharanya Reddy; Andrew N. Tyler; *PerkinElmer, Shelton, CT*
- ThP 034 **Simultaneous Determination of 74 kinds of pesticides in Chinese Herbal Medicine Listed in Chinese Pharmacopoeia (2015) by GPC-GC-MS/MS**; Yang Huiyan; Fan Jun; Huang Taohong; Shin-ichi Kawano; Yuki Hashi; *Shimadzu, Shanghai, China*
- ThP 035 **Improved Analysis of Allergens in Cosmetics by Cold EI GC/MS**; Sharanya Reddy; Thomas Dillon; Adam Patkin; Bill Hahn; *PerkinElmer, Shelton, CT*
- ThP 036 **Determination of Chemicals in Consumer Goods, Food Commodities and Drugs in a Rapid Method with Limited Sample Prep**; Louis Maljers<sup>1</sup>; Gordon van 't Slot<sup>2</sup>; <sup>1</sup>*Bruker, Fremont, Ca*; <sup>2</sup>*Bruker, Bremen, Germany*
- ThP 037 **Volatile & Semi-Volatile Profile Comparison of Whole Versus Cracked Versus Dry Homogenized Barley Grains by Direct Thermal Extraction GC/MS**; Ronald E. Shomo, II; Christopher Baker; John Manura; *Scientific Instrument Services, Ringoes, NJ*
- ThP 038 **Assessing the Thermal Stability and Degradation Characteristics of Chemical Warfare Nerve Agents via Pyrolysis GC-MS**; Jeffrey Mcquire<sup>1</sup>; John Carpin<sup>1</sup>; Matthew Parrish<sup>2</sup>; <sup>1</sup>*US Army ECBC, Aberdeen Proving Ground, MD*; <sup>2</sup>*LEIDOS, Gunpowder, MD*
- ThP 039 **Evaluation of Direct and Dopant-Assisted APLI in GC-MS Applications**; Faezeh Dousty<sup>1</sup>; Hendrik Kersten<sup>2</sup>; Thorsten Benter<sup>2</sup>; Rob O'Brien<sup>3</sup>; <sup>1</sup>*University of British Columbia Okanagan, Kelowna, BC, Canada*; <sup>2</sup>*University of Wuppertal, Wuppertal, Germany*; <sup>3</sup>*Supra Res & Dev, Kelowna, BC, Canada*
- ThP 040 **High Mass Accuracy Measurements and Elemental Composition Determination of Molecular Ions and Fragments of Pesticides with Single Quadrupole GC/MS Systems**; Ming Gu; Hongliang Xu; Yongdong Wang; *Cerno Bioscience, Norwalk, CT*
- ThP 041 **Rapid Analysis of Polychlorinated Biphenyls (PCBs) in Vegetables by QuEChERS-based Extraction and GPC-GCMS**; Xizhi Wang<sup>1</sup>; Shiheng Luo<sup>1</sup>; Feifei Tian<sup>1</sup>; Jun Fan<sup>2</sup>; Guixiang Yang<sup>1</sup>; Taohong Huang<sup>2</sup>; Shin-ichi Kawano<sup>2</sup>; Yuki Hashi<sup>2</sup>; <sup>1</sup>*Shimadzu Global COE, Shimadzu (China) Co.,Ltd., Beijing, China*; <sup>2</sup>*Shimadzu Global COE, Shimadzu (China) Co.,Ltd., Shanghai, China*
- ThP 042 **Characterization of Rose and Other Essential Oils and Synthetic Additives in them Using GC/MS with Cold EI Source**; Avinash Dalmia; Urs Steiner; *PerkinElmer, Shelton, CT*
- ThP 043 **Chemometric Methods for Botanical Classification of Chinese Honey According to Their Volatile Profiling by Solid-Phase Microextraction and Gas Chromatography-Mass**; Hui Chen<sup>1</sup>; Linghe Jin<sup>2</sup>; Chunlin Fan<sup>1</sup>; Guofang Pang<sup>1</sup>; Wenwen Wang<sup>3</sup>; Philip L. Wylie<sup>4</sup>; Joerg Riener<sup>5</sup>; Kumi Shiota Ozawa<sup>6</sup>; <sup>1</sup>*Chinese Academy of Inspection and Quarantine, Beijing, China*; <sup>2</sup>*Shandong Agriculture University, Tai'an, China*; <sup>3</sup>*Agilent Technologies, Beijing, China*; <sup>4</sup>*Agilent Technologies, Wilmington, DE*; <sup>5</sup>*Agilent Technologies, Waldbronn, Germany*; <sup>6</sup>*Agilent Technologies, Barueri, Brazil*
- ThP 044 **SIMAT: GC-SIM-MS Analysis Tool**; Mohammad R Nezami Ranjbar<sup>2</sup>; Cristina Di Poto<sup>1</sup>; Yue Wang<sup>2</sup>; Habtom Ressom<sup>1</sup>; <sup>1</sup>*Georgetown University, Lombardi Cancer Center, Washington, DC*; <sup>2</sup>*Virginia Tech, Arlington, VA*





- ThP 045 **A Spike-In Experiment for Assessment of GC-MS-based Analysis of Metabolites in Human Plasma;** Rency Varghese; Yue Luo; Cristina Di Poto; Mohammad R Nezami Ranjbar; Habtom Resson; *Georgetown University, Lombardi Cancer Center, Washington, DC*
- ThP 046 **Rapid Screening of Different Groups of Steroids by Multiple Selected Ion Monitoring in Biological Fluids;** Dick Bernhard; Bruno Vogt; Genevieve Escher; *Inselspital Nephrology, Hypertension, Bern, Switzerland*
- ThP 047 **New, Innovative Thermal Modulator Design for Two-Dimensional Gas Chromatography/ Mass Spectrometry Analysis;** Gaetano Stallone<sup>1</sup>; Massimiliano Saini Fasanotti<sup>2</sup>; Ilaria Ferrante<sup>2</sup>; <sup>1</sup>Volatome, Giovinazzo, Italy; <sup>2</sup>DANI Instruments SpA, Cologno Monzese, Italy
- ThP 048 **Evaluation of Methylisothiazolinone (MI) Extraction from Sunscreen using Supported Liquid Extraction prior to GC/MS Analysis;** Rhys Jones<sup>1</sup>; Lee Williams<sup>1</sup>; Alan Edgington<sup>1</sup>; Helen Lodder<sup>1</sup>; Adam Senior<sup>1</sup>; Geoff Davies<sup>1</sup>; Steve Jordan<sup>1</sup>; Claire Desbrow<sup>1</sup>; Victor vandell<sup>2</sup>; Elena Gairloch<sup>2</sup>; <sup>1</sup>Biotage GB Limited, Cardiff, Mid Glamorgan; <sup>2</sup>Biotage LLC, Charlotte, NC
- ThP 049 **Identification of High-Molecular Weight Brominated Flame Retardants in Environmental Samples using GC/Q-TOFMS;** Viorica Lopez-Avila; Jennifer Sanderson; *Agilent Technologies, Santa Clara, CA*
- ThP 050 **Open Probe Fast GC-MS – Real Time Analysis with Separation;** Aviv Amirav; Uri Keshet; Alexander Fialkov; Tal Alon; *Tel-Aviv University, Tel-Aviv, Israel*
- ThP 051 **GC Coupled to an Orbitrap-MS with a Novel Atmospheric Pressure Photoionization (APPI) Ion Source;** Joerg Hippler<sup>1</sup>; Oliver Knoop<sup>1</sup>; Amela Bronja<sup>1</sup>; Duxin Li<sup>1</sup>; Robert Ahrends<sup>2</sup>; Oliver J. Schmitz<sup>1</sup>; <sup>1</sup>University of Duisburg-Essen, Essen, Germany; <sup>2</sup>Leibniz-Institut für Analyt. Wissensch. - ISAS -, Dortmund, Germany
- ThP 052 **A Microfabricated Chromatographic Chip Integrated with a Peak-Refocusing Cold Trap for a Multi-dimensional GC/MS Analysis;** Sanggoo Kim; Sungmin Lim; *Korea Basic Sci. Institute, Seoul, South Korea*
- ThP 053 **Two-Dimensional Comprehensive Gas Chromatography Multi-Reflection Time-Of-Flight Mass Spectrometry: A Unique Tool to Merge Accurate Mass Information with High Chromatographic Resolution;** Thomas Groeger<sup>1</sup>; Ralf Zimmermann<sup>2</sup>; Benedikt Weggler<sup>1</sup>; Martin Sklorz<sup>2</sup>; Aimee Sutherland<sup>1</sup>; Juergen Wendt<sup>3</sup>; <sup>1</sup>Helmholtz Zentrum Muenchen, Oberschleissheim, Germany; <sup>2</sup>University of Rostock, Rostock, Germany; <sup>3</sup>LECO Instrumente GmbH, Moenchengladbach, Germany
- ThP 054 **Extending the Range of Compounds Amenable for GC-MS Analysis;** Alexander Fialkov; Tal Alon; Aviv Amirav; *Tel Aviv University, Tel Aviv, Israel*
- ThP 055 **Analysis of Metabolites in Human Plasma Using Stable Isotopes and Ultra-Fast GC-MS/MS System;** Yumi Unno<sup>1</sup>; Shuichi Kawana<sup>1</sup>; Yukihiro Kudo<sup>1</sup>; Takero Sakai<sup>1</sup>; Shin Nishiumi<sup>2</sup>; Masaru Yoshida<sup>2</sup>; Noriyuki Ojima<sup>1</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>Kobe University Graduate School of Medicine, Kobe, Japan
- ThP 056 **Automated Development of the Comprehensive Compound Database for Targeted MRM-based Metabolomics of Arabidopsis Plants using GC-MS/MS Technology;** Feroza K. Choudhury<sup>1</sup>; Dwain Cardona<sup>2</sup>; Amith Reddy<sup>1</sup>; Ron Mittler<sup>1</sup>; Vladimir Shulaev<sup>1</sup>; <sup>1</sup>University of North Texas, Denton, TX; <sup>2</sup>Thermo Fisher Scientific, Austin, TX
- ThP 057 **Screening for Hundreds of Pesticide Residues Using a GC/Q-TOF with an Exact Mass Pesticide Database in Various Food Matrices;** Joerg Riener<sup>1</sup>; Samanta Uclés<sup>2</sup>; Philip L. Wylie<sup>3</sup>; Wenwen Wang<sup>4</sup>; Jennifer Gushue<sup>5</sup>; Amadeo Fernández-Alba<sup>2</sup>; <sup>1</sup>Agilent Technologies, Waldbronn, Germany; <sup>2</sup>University of Almeria, Almeria, SPAIN; <sup>3</sup>Agilent Technologies, Wilmington, DE; <sup>4</sup>Agilent Technologies Co. Ltd, Beijing, China; <sup>5</sup>Agilent Technologies, Santa Clara, CA
- ThP 058 **A Comparison of ITEX Dynamic Headspace/GC/MS to Other Enrichment Techniques for Analysis of Flavoring Compounds;** Douglas Doster; *Aspen Research Corporation, New Germany, MN*
- ThP 059 **Determination of Residual Styrene Monomer in Copolymers by Headspace Solid Phase Microextraction Followed by GC/MS Using Isotope Dilution Calibration;** Dayna Turner; Andrei Stefanescu; *Novus International, Saint Charles, MO*
- ThP 060 **Software for Improved Sample Identification and Provision of Elemental Formula from Quadrupole based GC-MS Data;** Tal Alon<sup>1,2</sup>; Aviv Amirav<sup>1</sup>; <sup>1</sup>Tel Aviv University, Tel Aviv, Israel; <sup>2</sup>Afeka - Tel-Aviv Academic College of Engineering, Tel Aviv, Israel
- ThP 061 **Gas Chromatography Plasma-Assisted Reaction Chemical Ionization Mass Spectrometry: Quantification of Organohalogenes at High Sensitivity;** Haopeng Wang<sup>1</sup>; Carina Minardi<sup>1</sup>; Hamid Badie<sup>2</sup>; Kaveh Kahen<sup>2</sup>; Kaveh Jorabchi<sup>1</sup>; <sup>1</sup>Georgetown University, Washington, DC; <sup>2</sup>PerkinElmer Inc., Woodbridge, Canada

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- ThP 062 **Ion Mobility-Mass Spectrometry: A Novel Approach to Screening for Extractable and Leachable Components from Packaging Material;** Baiba Cabovska<sup>1</sup>; Eleanor Riches<sup>2</sup>; Cristina Nerin<sup>3</sup>; Margarita Aznar<sup>3</sup>; Pilar Alfaro<sup>3</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Waters Corporation, Wilmslow, UK; <sup>3</sup>CPS-University of Zaragoza, Zaragoza, Spain
- ThP 063 **Comprehensive Extractables Analysis of Medical Grade O-ring;** Dan Ewing<sup>1</sup>; Bill Hurley<sup>2</sup>; Andrew Feilden<sup>3</sup>; Michael Creese<sup>3</sup>; Kate Comstock<sup>4</sup>; Ekong Bassey<sup>4</sup>; John Schmelzel<sup>4</sup>; <sup>1</sup>Parker Hannifin O-ring Division, Lexington, KY; <sup>2</sup>Darcoid Nor-Cal Seal, Oakland, CA; <sup>3</sup>Smithers Rapra, Shawbury, UK; <sup>4</sup>Thermo Fisher Scientific, San Jose, CA
- ThP 064 **Characterization of Facial Cleansers by Kendrick Mass Defect Analysis using MALDI Spiral-TOFMS;** Kanae Teramoto<sup>1</sup>; Masaaki Ubukata<sup>2</sup>; Robert Cody<sup>2</sup>; Hiroaki Sato<sup>3</sup>; <sup>1</sup>JEOL Ltd., Akishima, Japan; <sup>2</sup>JEOL USA Inc., Peabody, MA; <sup>3</sup>Advanced Industrial Science and Technology (AIST), Tsukuba, Japan
- ThP 065 **Role of the Matrix in Fragile End-Group Cleavage upon MALDI of Synthetic Polymers;** Christophe Chendo; Trang N.T. Phan; Didier Gignes; Laurence Charles; *Aix-Marseille University, Marseille, France*
- ThP 066 **Trapped Ion Mobility Mass Spectrometry for Improved Additive Detection and Polymer Identification;** Jan Jordens<sup>1</sup>; Matthieu Besemer<sup>1</sup>; Ynze Mengerink<sup>1</sup>; Mark Ridgeway<sup>2</sup>; Melvin A. Park<sup>2</sup>; Maarten Honing<sup>1</sup>; <sup>1</sup>Resolve, Geleen, Netherlands; <sup>2</sup>Bruker Daltonics, Inc., Billerica, MA
- ThP 067 **Simultaneous Identification of Trace Organic Impurities in Purified Terephthalic Acid (PTA) by Ultra-High Performance Liquid Chromatography-Quadrupole Time-Of-Flight Mass Spectrometry;** Yidan Guo; *SINOPEC, Shanghai, China*
- ThP 068 **Structural Elucidation of Co-Polymer-Like Surfactants using MALDI Hi-Energy Collision Induced Dissociation;** Roberto Castangia<sup>2</sup>; Martin Resch Resch<sup>1</sup>; Matthew Openshaw<sup>2</sup>; Omar Belgacem<sup>2</sup>; <sup>1</sup>Shimadzu, Manchester, UK; <sup>2</sup>Shimadzu, Kratos, Manchester, UK
- ThP 069 **A Tandem Mass Spectrometry-Based Method to Assess the Architectural Purity of Synthetic Polymers: The Case of a Cyclic Poly lactide;** Thomas Josse<sup>1</sup>; Julien De Winter<sup>1</sup>; Philippe Dubois<sup>1</sup>; Olivier Coulembier<sup>1</sup>; Antony Memboeu<sup>2</sup>; Pascal Gerbaux<sup>1</sup>; <sup>1</sup>University of Mons, Mons, N/A; <sup>2</sup>Université de Bretagne Occidentale, Brest, France
- ThP 070 **Mass Spectrometry Characterization of Glycopolymers with Controlled Branching;** Sahar Sallam<sup>1</sup>; Chrys Wesdemiotis<sup>1</sup>; Liau Walter<sup>2</sup>; Andrea Kasko<sup>2</sup>; <sup>1</sup>The University of Akron, Akron, OH; <sup>2</sup>University of California, Los Angeles, CA

- ThP 071 **Matrix Assisted Laser Desorption Ionization Mass Spectrometry of Plasma Polymerized Styrene**; Lee Elliott; , *Carbondale, Illinois*
- ThP 072 **The Analysis of Cationic Polymers by MALDI-TOF MS**; Julie McGettrick; *University of Montana, Missoula, MT*
- ThP 073 **Characterization of Fatty Acid Methyl Ester Ethoxylates by Liquid Chromatography-Electrospray Ionization Mass Spectrometry**; Jian Li; Yan Liu; *Sinopec Shanghai Research Institute of Petrochemic, Shanghai, China*
- ThP 074 **Rapid Identification of Nylons by Temperature-Rising Direct Analysis in Real Time Mass Spectrometry (TR-DART-MS)**; Chikako Takei<sup>1</sup>; Kazumasa Kinoshita<sup>1</sup>; Takao Nishiguchi<sup>1</sup>; Haruo Shimada<sup>2</sup>; Katsuyuki Maeno<sup>2</sup>; Yasuo Shida<sup>3</sup>; <sup>1</sup>*BioChromato, Inc., Fujisawa, Japan*; <sup>2</sup>*Shiseido Research Center, Yokohama, Japan*; <sup>3</sup>*University of Yamanashi, Kofu, Japan*
- ThP 075 **Identification of Additives in a Molded Nitrile Rubber by PY/GCxGC/HRTOFMS**; Koji Okuda<sup>1</sup>; Jun Onodera<sup>1</sup>; Daniel Barabino<sup>2</sup>; Akihiko Kusai<sup>1</sup>; <sup>1</sup>*JEOL Ltd., Akishima, Japan*; <sup>2</sup>*JEOL USA, INC., Peabody, MA*
- ThP 076 **Density of Coordination Sites (DOCS): A Concept Reconciles Supramolecular Design, Complexity, Stability and Mass Spectrometry Characterization**; Bin Sun; Ming Wang; Alejandro Cisneros; Xiaopeng Li; *Texas State University, San Marcos, TX*
- ThP 077 **Improved Analysis of Ultra-High Mass Polymers in MALDI-TOF Mass Spectrometry**; Steffen M. Weidner<sup>1</sup>; Stefan Johannes Gabriel<sup>1</sup>; Ulrich Panne<sup>1</sup>; Robert Steinhoff<sup>2</sup>; Renato Zenobi<sup>2</sup>; Clemens Schwarzwinger<sup>3</sup>; <sup>1</sup>*Federal Institute f. Material Research and Testing, Berlin, Germany*; <sup>2</sup>*ETH Zurich, Zurich, Switzerland*; <sup>3</sup>*Johannes Kepler Universität, Linz, Austria*
- ThP 078 **Multidimensional Mass Spectrometry Analysis of Polyglycerol**; Ahlam Alalwiat; Sahar Sallam; Chrys Wesdemiotis; *The University of Akron, Akron, U.S.A*
- ThP 079 **Citric Acid-Capped Iron Oxide Nanoparticles as an Effective MALDI Matrix for Polymer Analysis**; Qiaoli Liang; Jennifer Sherwood; Thomas Macher; Yuping Bao; Carolyn J. Cassidy; *University of Alabama, Tuscaloosa, AL*
- ThP 080 **Preparation of Candidate Standard Reference Material (SRM) 2860 Restricted Substances in Polyvinyl Chloride (PVC) and Measurement of Phthalates by Gas Chromatography/Mass Spectrometry**; Bruce A. Benner, Jr.<sup>1</sup>; David P. Owen<sup>2</sup>; Katherine Stahl<sup>2</sup>; Kristi Utech<sup>2</sup>; Leena Pitkänen<sup>1</sup>; André M. Striegel<sup>1</sup>; <sup>1</sup>*NIST, Gaithersburg, MD*; <sup>2</sup>*BASF, Pasadena, TX*
- ThP 081 **Characterisation of a Polydisperse Cationic Polyethylenimine (PEI) Lipid using MALDI-MS, LC-ELSD-TOFMS, SEC-MALS, NMR and Solid State NMR**; Lena von Sydow; Johan Broddefalk; Gunnar Grönberg; Pernilla Korsgren; Sara Richardson; Anna Svensk Ankarberg; Staffan Schantz; *AstraZeneca R&D, Mölndal, Sweden*
- ThP 082 **Enrichment and MALDI-MS Analysis of Peptides by Amphiphilic Homopolymer-Based Reverse Micelle with Different Functionalities**; Bo Zhao; Feng Wang; Sankaran Thayumanavan; Richard Vachet; *University of Massachusetts Amherst, Amherst, MA*
- ThP 083 **Simplification of Pharmaceutically Relevant Polymer Mass Spectra via Gas-Phase Ion/Ion Reactions with Carborane Anions**; Carl Luongo<sup>1</sup>; Stella Betancourt<sup>1</sup>; Steven Cummings<sup>2</sup>; Christopher Reed<sup>2</sup>; Scott McLuckey<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*University of California Riverside, Riverside, CA*
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- ThP 084 **Automatic Optimization of MS and MS/MS Assays for Dilute Samples or Weak Transitions**; Bennett Kalafut; *Thermo Fisher Scientific, San Jose, CA*
- ThP 085 **Investigation for Gas-phase Fragmentation of N-phenyl Ferrocene Imine Derivatives Studied by Mass Spectrometry**; Yawen Mo; , *Hangzhou, P.R. China*
- ThP 086 **Low Energy Collision-Induced Dissociation Tandem Mass Spectrometry of Metal-Yersiniabactin Complexes: An Empirical and Theoretical Study**; Daryl Giblin; Eun-Ik Koh; Jan R. Crowley; Michael Gross; Jeffrey P. Henderson; *Washington University, St Louis, MO*
- ThP 087 **Ambulation of Incipient Proton, and Elimination of an Alcohol or Alkene during Gas-phase Fragmentation of Protonated Alkyl Dihydrocinnamate**; Sihang Xu; Athula Attygalle; *Stevens Institute of Technology, Hoboken, NJ*
- ThP 088 **Utilizing Gas-phase Fragmentation Chemistry for Multi-component Mixture Analysis**; Maha T. Abutokaikah; Benjamin J. Bythell; *Univ. of Missouri-St. Louis, St. Louis, MO*
- ThP 089 **Formation of Superoxide [O<sub>2</sub><sup>-</sup>] Anion Adducts from Amides under Atmospheric Pressure Helium-Plasma Ionization (HePI) Conditions**; Isra Hassan; Spencer Pinto; Athula Attygalle; *Stevens Institute of Technology, Hoboken, NJ*
- ThP 090 **Hydrogen Attachment Dissociation (HAD): A Novel Fragmentation Mass Spectrometry for Singly and Multiply Charged Peptide Ions**; Hidenori Takahashi<sup>1</sup>; Sadanori Sekiya<sup>1</sup>; Takashi Nishikaze<sup>1</sup>; Kei Koderai<sup>1</sup>; Shinichi Iwamoto<sup>1</sup>; Motoi Wada<sup>2</sup>; Koichi Tanaka<sup>1</sup>; <sup>1</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>2</sup>*Doshisha University, Kyotanabe, Japan*
- ThP 091 **Impact of Cobalt Oxidation State and  $\beta$  Ligand on Ion Formation in Electrospray Ionization and Collision-Induced Dissociation of Cobalamins**; Liqiong Fang; Almary Chacon; Peifeng Hu; *Baxter Healthcare Corporation, Round Lake, IL*
- ThP 092 **Characterization of End Group Functionalized Poly(N-isopropylacrylamides) by Using Multiple ETD/CAD Stages**; Selim Gerislioglu; Chrys Wesdemiotis; *The University of Akron, Akron, OH*
- ThP 093 **Investigation for Gas-phase Fragmentation of N-phenyl Ferrocene Carboxamides in ESI Mass Spectrometry**; Linji Chen; *Hangzhou, P.R. China*
- ThP 094 **Proton Transfers in the Fragmentation of Protonated N-benzylbenzamides in Electrospray Ionization Mass Spectrometry**; Yunfeng Chai; Yuanjiang Pan; *Zhejiang University, Hangzhou, China*
- ThP 095 **Investigation for Gas-phase Fragmentation of 3-Idolphenyl Phenyl Sulfides by APCI Mass Spectrometry**; Chenlu Wang; , *Hangzhou, China*
- ThP 096 **Dissociative Benzyl Cation Transfer in the Fragmentation of Protonated 3-[(5-aryl-1,3,4-oxadiazol-2-yl)methyl]benzo[d]thiazol(2H)-ones**; Ye Wang; , *Hangzhou, China*
- ThP 097 **Carboranes: Gas Phase Properties of Large Caged Molecules**; Omar Hamdy; Ryan R. Julian; *University of California, Riverside, Riverside, CA*
- ThP 098 **ESI-Induced Oxygen Transfer from Nitro Group to Alkyl Chain in N-alkyl-2-nitroanilines**; George Mathai<sup>1</sup>; June Cyriac<sup>1</sup>; Justin Paulose<sup>1</sup>; Daryl Giblin<sup>2</sup>; Michael Gross<sup>2</sup>; <sup>1</sup>*Sacred Heart College, Kochi, India*; <sup>2</sup>*Department of Chemistry, Washington University, St. Louis, MO*
- ThP 099 **Probing Dissociation of Collisionally Excited Non-Covalent Complexes by Energy-Resolved CID and Computational Chemistry**; Glenn Carroy<sup>1</sup>; Vincent Lemaury<sup>1</sup>; Julien De Winter<sup>1</sup>; Denis Morsa<sup>2</sup>; Jérôme Cornil<sup>1</sup>; Edwin De Pauw<sup>2</sup>; Pascal Gerbaux<sup>1</sup>; <sup>1</sup>*UMONS, Mons, Belgium*; <sup>2</sup>*ULG, Liège, Belgium*
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- ThP 161 **High Resolution Silver Assisted LDI Imaging MS to Monitor the Molecular Composition of Latent Fingermarks towards Forensic Applications;** Nidia Lauzon<sup>1</sup>; Martin Dufresne<sup>1</sup>; Vinita Chauhan<sup>2</sup>; Pierre Chaurand<sup>1</sup>; <sup>1</sup>University of Montreal, Montreal, Canada; <sup>2</sup>Health Canada, Ottawa, Canada
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- ThP 163 **Direct Analysis of New Psychoactive Substances by Portable Mass Spectrometer;** Kazushige Nishimura<sup>1</sup>; Masuyoshi Yamada<sup>1</sup>; Akihito Kaneko<sup>1</sup>; Hidetoshi Morokuma<sup>2</sup>; Fumiyo Kasuya<sup>3</sup>; Yukiko Nakazono<sup>4</sup>; Kenji Tsujikawa<sup>4</sup>; Yuko T. Iwata<sup>4</sup>; Hiroyuki Inoue<sup>4</sup>; <sup>1</sup>Hitachi Ltd., Tokyo, Japan; <sup>2</sup>Hitachi High-Technologies Co., Hitachinaka, Japan; <sup>3</sup>Kobegakuin University, Kobe, Japan; <sup>4</sup>National Research Institute of Police Science, Kashiwa, Japan
- ThP 164 **Femtogram Detection of 11-nor-9 carboxy-THC in Methanolic Solutions Using an Integrated Microfluidics MS System;** Rob Lee<sup>1</sup>; Gregory Roman<sup>2</sup>; Jim Murphy<sup>2</sup>; Michelle Wood<sup>1</sup>; <sup>1</sup>Waters Corporation, Wilmslow, UK; <sup>2</sup>Waters Corporation, Milford, USA
- ThP 165 **MALDI-TOF MS to Identify Unknown Tapes;** Lindsey Rasmussen; Evgenia Tisdale; Rohana Liyanage; Charles L. Wilkins; University of Arkansas, Fayetteville, AR
- ThP 166 **Enhancing Workplace Drug Testing by Multi-Column Dilute and Shoot LC-MS/MS;** David R. Baker<sup>1</sup>; Christopher Titman<sup>2</sup>; Paul Powles<sup>3</sup>; <sup>1</sup>Shimadzu, Manchester, UK; <sup>2</sup>Shimadzu UK Limited, Cambridge, UK; <sup>3</sup>ESG, Burton-on-Trent, UK
- ThP 167 **Optimization of LC-ESI (+)-MS-TOF Analysis of Tropane, Harmala and Pyrrolizidine Alkaloids Isolated by MSPD from Tropical Plants Grown in Colombia;** Elena Stashenko; Fausto Prada; Jessica Mejia; Lady Sierra; Cristian Oliveros; Corina Bernal; John Rodriguez; Jairo René Martínez; Universidad Industrial de Santander, Bucaramanga, Colombia
- ThP 168 **Fast and Confident Identification of Drugs and Their metabolites using Ion Trap LC-MSn Analysis and a Library of >4,500 Compounds;** Birgit Schneider<sup>1</sup>; Andrea Kiehne<sup>1</sup>; Markus Meyer<sup>1</sup>; Sebastian Goetz<sup>1</sup>; Steve Fannin<sup>2</sup>; Carsten Baessmann<sup>1</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup>Bruker Daltonics, Billerica, MA
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- ThP 170 **Identification of Drugs Using a Field Deployable DART-ITMS with On Board Library;** Berk Oktem; Alexander S. Misharin; Konstantin Novoselov; Vladimir M. Doroshenko; *MassTech Inc., Columbia, MD*
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- ThP 172 **High Sensitivity Analysis Of Opioids In Oral Fluid Using Integrated Microfluidics;** Gregory Roman<sup>1</sup>; Robert Lee<sup>2</sup>; James Murphy<sup>1</sup>; Michelle Wood<sup>2</sup>; Jeff Goshawk<sup>3</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Waters Corporation, Wilmslow, UK; <sup>3</sup>Waters, Manchester, N/A
- ThP 173 **Database Search Strategy for Proteomic Characterization of Unknown Samples: A Clostridium botulinum Case Study;** Andy Lin; Eric Merkley; Brooke Kaiser; Karen Wahl; *Pacific Northwest National Laboratory, Richland, WA*
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- ThP 324 **Phosphorylation Stoichiometry Measurement on a Large Scale by Motif-Targeting Quantitative Proteomics;** Chia-Feng Tsai<sup>2</sup>; Yi Ting Wang<sup>2</sup>; Yu-Ju Chen<sup>2</sup>; Yasushi Ishihama<sup>1</sup>; <sup>1</sup>Kyoto University, Kyoto, Japan; <sup>2</sup>Academia Sinica, Taipei, Taiwan
- ThP 325 **Quantitative Label-Free Phosphoproteomics for Understanding Biological Pathways in Chlamydomonas reinhardtii;** Emily Werth; William Slade; Leslie Hicks; *University of North Carolina, Chapel Hill, NC*
- ThP 326 **Correlating Polo-like Kinase 1 (Plk1) Kinetochores Localization with Kinase Function using Quantitative Phosphoproteomics;** Gregory K. Potts; Robert F. Lera; Alex Hebert; Michael S. Westphall; Mark E. Burkard; Joshua J. Coon; *University of Wisconsin, Madison, WI*
- ThP 327 **Striatal Global Phosphoproteomics Analysis of the zQ175 Huntington's Disease Mouse Model following PDE10A Inhibition;** J. Nikolaj Dybowski<sup>1</sup>; Vahri Beaumont<sup>2</sup>; Andreas Tebbe<sup>1</sup>; Christoph Schaab<sup>1</sup>; Sarah Elschenbroich<sup>1</sup>; Daniel Lavery<sup>2</sup>; Christopher Schmidt<sup>3</sup>; Ignacio Munoz-Sanjuan<sup>2</sup>; <sup>1</sup>Evotec (München) GmbH, Munich, Germany; <sup>2</sup>CHDI Foundation, Los Angeles, CA; <sup>3</sup>Pfizer Neuroscience Research Unit, Cambridge, MA
- ThP 328 **Individualized Tissue Analysis for EGFR-dependent Phosphoproteomics Signature in Non-small-cell Lung Cancer;** Yi Ting Wang<sup>1</sup>; Chia-Feng Tsai<sup>1</sup>; Pei-Yi Lin<sup>1</sup>; Hsuan-Yu Chen<sup>2</sup>; Chia-Jung Yu<sup>3</sup>; Pan-Chyr Yang<sup>4</sup>; Yu-Ju Chen<sup>1</sup>; <sup>1</sup>Institute of Chemistry, Academia Sinica, Taipei, Taiwan; <sup>2</sup>Institute of Statistical Science, Academia Sinica, Taipei, Taiwan; <sup>3</sup>College of Medicine, Chang Gung University, Tao-Yuan, Taiwan; <sup>4</sup>College of Medicine, National Taiwan University, Taipei, Taiwan
- ThP 329 **CaMKII Phosphorylation of Na<sub>v</sub>1.5 on S516 in Human Heart Failure and Novel Phosphorylation Sites Identified by Label-Free Quantitative Mass Spectrometry;** Anthony Herren<sup>1</sup>; Darren Weber<sup>1</sup>; Robert Rigor<sup>1</sup>; Kenneth Margulies<sup>2</sup>; Brett Phinney<sup>1</sup>; Donald Bers<sup>1</sup>; <sup>1</sup>University of California, Davis, Davis, CA; <sup>2</sup>University of Pennsylvania, Philadelphia, PA
- ThP 330 **Regulation of Phosphorylation Mediated Signaling Events in O-GlcNAcase-inhibited or Bone Morphogenetic Protein (BMP)-stimulated Osteoblasts;** Alexis Nagel;

- ThP 331 Jennifer R Bethard; Benjamin Neely; Lauren Ball; *Department of Pharmacology, MUSC, Charleston, SC*  
**Phosphoproteomic Profiling of Phosphorylation Stoichiometry in Kinase-Mediated *in vitro* Phosphorylation Reaction**; Pasrawin Taechawattananant; Dai Sakamoto; Masaki Wakabayashi; Naoyuki Sugiyama; Yasushi Ishihama; *Kyoto University, Kyoto, Japan*
- ThP 332 **Quantitative Analysis of Large Phosphopeptide Datasets using Proteome Discoverer 2.0**; David Horn<sup>1</sup>; Ilyas Singec<sup>2</sup>; Laurence Brill<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Sanford-Burnham Medical Research Institute, La Jolla, CA
- ThP 333 **Transient Phosphokinetics Tracked by Data-independent Acquisition with High-density Time Course**; Rong Zeng; Qing-Run Li; Hong-Wen Zhu; Shi-Sheng Wang; *Shanghai Institutes for Biological Sciences, Shanghai, China*
- ThP 334 **Nano Flow LC-MS Analyses of Insulin Receptor Site-specific Phosphorylation Induced by Insulin Lispro and PEGylated Insulin Lispro**; Zhongping Liao; Jason Tang; John Beals; *Eli Lilly and Company, Indianapolis, IN*
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- ThP 336 **Phosphorylation Dynamics of PTHR Signaling in Osteoblasts with Functionally Selective Agonists**; Grace Williams; Jennifer Bethard; Mary Berkaw; Louis Luttrell; Lauren Ball; *Medical Univ of S Carolina, Charleston, SC*
- ThP 337 **Relative Phosphoproteomics Quantitation for Pathogenic *Escherichia coli* Strains using Orbitrap Fusion Mass Spectrometer**; Rabih Jabbour<sup>1</sup>; Raja Sekhar Nirujogi<sup>2</sup>; Mary Wade<sup>1</sup>; Akhilesh Pandey<sup>2</sup>; <sup>1</sup>ECBC, Apg, MD; <sup>2</sup>Johns Hopkins University School of Medicine, Baltimore, MD
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- ThP 339 **Total Protein Profiling Employing a Novel Protein Fractionation Method Combined with Tandem Mass Tag Labeling**; Charles Farnsworth<sup>1</sup>; Matthew P. Stokes<sup>1</sup>; Hongbo Gu<sup>1</sup>; Xiaoying Jia<sup>1</sup>; Sadaf Hoda<sup>2</sup>; Bryan Spencer<sup>2</sup>; Ezra S. Abrams<sup>2</sup>; Christian Boles<sup>2</sup>; Jeffrey C. Silva<sup>1</sup>; <sup>1</sup>Cell Signaling Technology, Danvers, MA; <sup>2</sup>Sage Science, Beverly, MA
- ThP 340 **Efficient Method for the Determination of a 28 Amino Acid Peptide in Human EDTA K2 Plasma by LCMSMS**; Carine Lévesque; Philippe Bélanger; Marie-Josée Marcoux; Nadine Boudreau; Ann Lévesque; *InVentiv Health Clinical, Québec, Canada*
- ThP 341 **Evaluation and Optimization of Waters IonKey/MS System for High-Throughput and High Sensitivity Quantitative Analysis for Insulin Analogues in Biological Matrices**; Hsuan-Shen Chen<sup>1</sup>; Bernard Choi<sup>1</sup>; Yang Xu<sup>2</sup>; Dina Goykhman<sup>2</sup>; Lucinda Cohen<sup>1</sup>; <sup>1</sup>Merck Research Laboratories, Rahway, NJ; <sup>2</sup>Merck Research Laboratories, West Point, PA
- ThP 342 **Increasing Reproducibility and Performance of Targeted Quantitation Using HD-PRM**; Michael Blank<sup>1</sup>; Bruno Domon<sup>2</sup>; Andreas FR Huhmer<sup>1</sup>; Antoine Lesur<sup>3</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Luxembourg Clinical Proteomics, Strassen, Luxembourg; <sup>3</sup>Luxembourg Clinical Proteomics Center, Strassen, N/A
- ThP 343 **Low Attomole Limit of Quantification on a Q-q-OT-IT Hybrid Mass Spectrometer**; Romain Huguët; Michael Blank; Seema Sharma; Nina Soltero; Vlad Zabrouskov; *Thermo Fisher Scientific, San Jose, CA*
- ThP 344 **Degradation of Synthetic Peptides Caused by Thermal Denaturation during Targeted Proteomics Sample Preparation and Its Impact on LC-MS/MS Assay Accuracy**; Bob Xiong; Lynn Garcowski; Lori Wright; Brian Nofsinger; Mike Allen; *Tandem Labs - RTP, Durham, NC*
- ThP 345 **TMT Ratio Decompression – MultiNotch MS3 or fractionation?** Benjamin Ruprecht<sup>1</sup>; Dominic Helm<sup>1</sup>; Jana Zecha<sup>1</sup>; Elena Kunold<sup>2</sup>; Stephan Sieber<sup>2</sup>; Bernhard Kuster<sup>1</sup>; <sup>1</sup>Technische Universität München, Freising, Germany; <sup>2</sup>Technische Universität München, Garching, Germany
- ThP 346 **Development of a High Sensitivity SPE-LC-MS/MS Assay for the Quantification of Glucagon in Human Plasma using an Integrated Microfluidic Device**; Erin E. Chambers; Mary Lame; Markus Wanninger; *Waters Corporation, Milford, MA*
- ThP 347 **Performance of a 120-plex Immuno-Multiple Reaction Monitoring Mass Spectrometry Assay in Plasma of Patients with Cardiovascular Disease**; Paul Ippoliti; Eric Kuhn; D. R. Mani; Hasmik Keshishian; Michael Burgess; Jacob D. Jaffe; Steven A. Carr; *The Broad Institute of MIT and Harvard, Cambridge, MA*
- ThP 348 **An Immunocapture-LC-MS/MS Workflow for Adalimumab (Humira) and Infliximab (Remicade) Quantitation in Human Plasma**; Witold Woroniecki; Lei Xiong; Kelli Jonakin; Shaw Xia; Suma Ramagiri; Hua-Fen Liu; *Sciex, Redwood City, CA*
- ThP 349 **HPLC-MS/MS Quantification of Targeted Neuropeptides in Tac1-/- Mouse Spinal Cords Reveals Significantly Lower Concentrations of Opioid Peptides**; Mouna Saidi; Francis Beaudry; *Université de Montréal, St-Hyacinthe, Canada*
- ThP 350 **A Sensitive LC-MS/MS Method for the Quantification of a Small 9-Amino Acid Therapeutic Peptide in Clinical Plasma**; Nader Youssef; Weixing Sun; John Chapdelaine; Adrien Musuku; *Pharmascience, Montreal, Canada*
- ThP 351 **Automated High Throughput Peptide and Protein MRM Optimization and On-Column HPLC Screening for Pharmaceutical Method Development**; Ian Moore; Suma Ramagiri; *AB SCIEX, Concord, Canada*
- ThP 352 **Determination of Relative Expression Levels of HLA Class-I Proteins using Immunoprecipitation in Combination with Selected Ion Monitoring Mass Spectrometry**; Zhaojing Meng; Richard Apps; Gregory Del Prete; Jeffrey Lifson; Mary Carrington; Ming Zhou; *Frederick National Laboratory for Cancer Research, Frederick, MD*
- ThP 353 **Site-specific Quantitation of the Lysine Acetylation Degree: A Generic MS2-based Method using <sup>13</sup>C<sub>4</sub>-acetyl Labeling and Unspecific Proteases**; Rasha ElBashir<sup>1</sup>; Jens T. Vanselow<sup>1</sup>; Amelie Kraus<sup>2</sup>; T. Nicolai Siegel<sup>2</sup>; Andreas Schlosser<sup>1</sup>; <sup>1</sup>Rudolf Virchow Center, Würzburg, Germany; <sup>2</sup>Research Center for Infectious Diseases, Würzburg, Germany
- ThP 354 **Mass Spectrometry Based Detection of Peptide Changes in Learned Drug Associations**; Sarah Dowd; Martina Mustroph; Elena Romanova; Bruce Southey; Justin Rhodes; Jonathan Sweedler; *University of Illinois at Urbana Champaign, Urbana, IL*
- ThP 355 **Quantitative Analysis of Neuropeptides using *in vivo* Microdialysis Coupled with UHPLC Triple-Quadrupole Mass Spectrometry**; Matthew Buczynski<sup>1</sup>; Yanan Yang<sup>2</sup>; Luis Natividad<sup>1</sup>; Andy Gieschen<sup>3</sup>; Loren Parsons<sup>1</sup>; <sup>1</sup>The Scripps Research Institute, La Jolla, CA; <sup>2</sup>Agilent Technologies, Inc, Santa Clara, CA; <sup>3</sup>Agilent Technologies, La Jolla, CA
- ThP 356 **A Sensitive LC-MS/MS Method for Quantitation of Glucagon in Human Plasma**; Witold Woroniecki; Lei Xiong; Kelli Jonakin; Rahul Baghla; Suma Ramagiri; Hua-Fen Liu; *Sciex, Redwood City, CA*



- ThP 357 **Impact Assessment of Methionine Oxidation on the Quantitative Analysis of a Model Therapeutic Peptide by Trypsin Digestion and LC-HRMS**; Louis-Philippe Morin; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*
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- ThP 359 **Use of High Resolution Mass Spectrometry (HRMS) for Synthetic Peptide and Oligonucleotide Mapping with Data-Independent Acquisition**; Man-Yu Zhang<sup>1</sup>; Yanan Yang<sup>2</sup>; Shan-An Chan<sup>3</sup>; <sup>1</sup>*Agilent, Shanghai, China*; <sup>2</sup>*Agilent, Santa Clara, CA*; <sup>3</sup>*Agilent, Taipei, Taiwan*
- ThP 360 **Derivatization of Singly Charged, Hydrophobic Peptides Improves MS2 Spectra**; Melissa Budelier<sup>1</sup>; ZiWei Chen<sup>1</sup>; Jason Held<sup>1,2</sup>; Reid Townsend<sup>2</sup>; Alex Evers<sup>1</sup>; <sup>1</sup>*Dept of Anesthesiology, Washington University, St. Louis, MO*; <sup>2</sup>*Internal Medicine, Washington University, St. Louis, MO*
- ThP 361 **N-terminal Charge-Driven de novo Sequencing by using ASDF-incorporated Curved Field Reflectron**; Yuzo Yamazaki<sup>1</sup>; Keisuke Shima<sup>1</sup>; Atsushi Kitanaka<sup>2</sup>; Masahiro Miyashita<sup>2</sup>; Hisashi Miyagawa<sup>2</sup>; <sup>1</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>2</sup>*Graduate School of Agriculture, Kyoto University, Kyoto, Japan*
- ThP 362 **De novo Sequencing-Assisted Peptide Mapping for Quantitative Analysis of Peptide Variants**; Katherine Tran<sup>1</sup>; Cheryl Lichti<sup>2</sup>; Baozhen Shan<sup>1</sup>; Carol Nilsson<sup>2</sup>; <sup>1</sup>*Bioinformatics Solutions Inc., Waterloo, Canada*; <sup>2</sup>*UTMB Cancer Center, University of Texas, Galveston, TX*
- ThP 363 **Protease-Containing Membranes for Monoclonal Antibody Digestion Prior to MS Analysis**; Yongle Pang<sup>1</sup>; Gavin Reid<sup>2</sup>; Merlin Bruening<sup>1</sup>; <sup>1</sup>*Michigan State University, East Lansing, MI*; <sup>2</sup>*University of Melbourne, Parkville, Australia*
- ThP 364 **Characterization of Endoproteolytic Processing of Dynorphins using Brain and Spinal Cord Cellular Fractions and Mass Spectrometry**; Alberto Ruiz; Francis Beaudry; *Université de Montréal, St-Hyacinthe, Canada*
- ThP 365 **OrbiTrap for the de novo Sequencing of Non Tryptic Skin Peptides of Slovenian Brown Frogs *Rana latastei* and *Rana temporaria***; Tatiana Samgina<sup>1</sup>; Konstantin Artemenko<sup>2</sup>; Bergquist Jonas<sup>2</sup>; Polonca Trebse<sup>3</sup>; Gregor Torkar<sup>4</sup>; Maria Tolpina<sup>1</sup>; Albert T. Lebedev<sup>1</sup>; <sup>1</sup>*Moscow State University, Moscow, Russian Federation*; <sup>2</sup>*Uppsala University, Uppsala, Sweden*; <sup>3</sup>*Ljubljana University, Slovenja, Ljubljana, Slovenia*; <sup>4</sup>*University of Nova Gorica, Nova Gorica, Slovenia*
- ThP 366 **Disulfide Linked Linear and Cyclic Peptides Automatically Assigned Using Nominal and Exact Mass ESI-MS/MS Data and the MASSPEC Algorithm**; Marshall M. Siegel<sup>1</sup>; Gary Walker<sup>1</sup>; Eugene F. Ciccimaro<sup>2</sup>; Serhiy Hnatyshyn<sup>2</sup>; Asoka Ranasinghe<sup>2</sup>; <sup>1</sup>*MS Mass Spec Consultants, Fair Lawn, NJ*; <sup>2</sup>*Bristol-Myers Squibb, Princeton, NJ*
- ThP 367 **Identifying Sequence Variants by an Integrated Mass Spectrometric and Informatics Workflow**; Stephane Houel<sup>1</sup>; Barry Dyson<sup>2</sup>; Rose Lawler<sup>1</sup>; Weibin Chen<sup>1</sup>; <sup>1</sup>*Waters Corp, Milford, MA*; <sup>2</sup>*Waters corp., Wimslow, UK*
- ThP 368 **Acidic Peptide Sequence Effects on Metal Attachment and Electron Transfer Dissociation Fragmentation**; Juliette J. Comodore; Carolyn J. Cassidy; *The University of Alabama, Tuscaloosa, AL*
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- ThP 372 **Development of Methods with Self-Optimizing QTOF MS/MS for Detection and de novo Sequence Verification of Synthetic Peptide in Biopharmaceutical Applications**; Chensong Pan<sup>1</sup>; Sawyen Ow<sup>2</sup>; <sup>1</sup>*Bruker (Beijing) Scientific Technology Co. Ltd., Beijing, China*; <sup>2</sup>*Bruker Daltonics Pte Ltd, Singapore, Singapore*
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- ThP 374 **3D High Resolution Mass Mapping as Screening Tool for the Discovery of Cysteine-Containing Peptides from Complex Biological Mixtures**; Martijn W. Pinkse; Luuk N. Van Oosten; Mervin M. Pieterse; Peter D. Verhaert; *Delft University of Technology, Delft, Netherlands*
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- ThP 376 **A Novel 6x5 Peptide Mixture for Instrument Performance Monitoring and Method Optimization**; Michael Rosenblatt<sup>1</sup>; Ethan Strauss<sup>1</sup>; Joshua Beri<sup>2</sup>; Michael Bereman<sup>3</sup>; Marjeta Uhr<sup>2</sup>; <sup>1</sup>*Promega Corp, Madison, WI*; <sup>2</sup>*Promega, Madison, WI*; <sup>3</sup>*North Carolina State University, Raleigh, NC*
- ThP 377 **Use of Alternative Non-Ionic Surfactants for Improved Efficiency of in situ Tryptic Proteolysis**; Ekta Patel<sup>1</sup>; Malcolm Clench<sup>1</sup>; Peter Marshall<sup>2</sup>; Andy West<sup>2</sup>; Nathan Marshall<sup>1</sup>; Simona Francese<sup>1</sup>; <sup>1</sup>*BMRC Sheffield Hallam University, Sheffield, UK*; <sup>2</sup>*GlaxoSmithKline, Stevenage, UK*
- ThP 378 **LC/ESI-MSMS Determination of Botulinum A Toxicity Inhibition by Various Hydroxamates**; Kathleen Housman; Matthew Levit; Joshua Emory; Michael Adler; Jonathan Oyler; *USAMRICD, Aberdeen Proving Ground, MD*
- ThP 379 **Determination of Antioxidative Peptide by HPLC-screen Printed Electrode-Nanospray Ionization Mass Spectrometry**; Ya-Chen Hung; Kuo-Lung Ku; *National Chiayi University, Chiayi City, Taiwan*
- ThP 380 **Sample Preparation using Membrane Separation Technique Significantly Increases the Peptide Identification from Soy Protein Hydrolysates via LC-MS**; Parthasarathi Ghosh; Alexandria Malam; *DuPont Nutrition & Health, St. Louis, MO*
- ThP 381 **LC-MS/MS Analysis of Misincorporation of Beta Methylnorleucine for Leucine and Isoleucine in Monoclonal Antibodies Produced in E. Coli**; Benjamin Moore; *Genentech, South San Francisco, CA*
- ThP 382 **Mass Spectrometric Investigation of Neuropeptidomic Alteration in Food Intake**; Jingxin Wang<sup>1</sup>; Hui Ye<sup>1,2</sup>; Fengfei Ma<sup>1</sup>; Ryan Selleck<sup>1</sup>; Brian Baldo<sup>1</sup>; Lingjun Li<sup>1</sup>; <sup>1</sup>*UW-Madison, Madison, WI*; <sup>2</sup>*China Pharmaceutical University, Nanjing, China*
- ThP 383 **Balancing Speed, Sample Complexity and Data Quality in Proteomics Applications on a benchtop Quadrupole-Orbitrap mass spectrometer**; Tabiwang N. Arrey; Eugen Damoc; Yue Xuan; Kerstin Strupat; Thomas Moehring;

- Markus Kellmann; *Thermo Fisher Scientific, Bremen, Germany*
- ThP 384 **Peptide Capture using Self-Assembled Monolayers on Gold for Mass Spectrometric Analysis;** [Helen Robinson](#)<sup>1</sup>; Anne Routledge<sup>1</sup>; Jane Thomas-Oates<sup>1,2</sup>; <sup>1</sup>*Department of Chemistry, University of York, York, UK;* <sup>2</sup>*Centre of Excellence in Mass Spectrometry, York, UK*
- ThP 385 **Mass Spectral Measurement of Feeding-Related Neuropeptide Secretion in Crustacean via *in vivo* Microdialysis;** [Zhidan Liang](#)<sup>1,2</sup>; Lingjun Li<sup>1,2</sup>; <sup>1</sup>*University of Wisconsin, Madison, WI;* <sup>2</sup>*University of Wisconsin, Madison, WI*
- ThP 386 **Homology-driven *de novo* Peptidomics of Genetically Unannotated Animal Species;** [Elena V. Romanova](#)<sup>1</sup>; Stanislav S Rubakhin<sup>1</sup>; Ioanna Ntai<sup>2</sup>; Bruce R Southey<sup>1</sup>; Justin S Rhodes<sup>1</sup>; Neil L. Kelleher<sup>2</sup>; Jonathan Sweedler<sup>1</sup>; <sup>1</sup>*University of Illinois, Urbana, IL;* <sup>2</sup>*Northwestern University, Evanston, IL*
- ThP 387 **Multifaceted Mass Spectrometric Profiling of Neuropeptides in *Callinectes sapidus* during Hypoxia;** [Amanda Buchberger](#)<sup>1</sup>; Lingjun Li<sup>1,2</sup>; <sup>1</sup>*Department of Chemistry, University of Wisconsin, Madison, WI;* <sup>2</sup>*School of Pharmacy, University of Wisconsin, Madison, WI*
- ThP 388 **Introducing Peptidomics to Migraine Research: Neuropeptidomics Study of Migraine and Opioid Induced Hyperalgesia Related Regions through Liquid Chromatography Mass Spectrometry;** [Ning Yang](#)<sup>1</sup>; Elena Romanova<sup>1</sup>; Stanislav Rubakhin<sup>1</sup>; Amynah Pradhan<sup>2</sup>; Jonathan Sweedler<sup>1</sup>; <sup>1</sup>*University of Illinois at Urbana Champaign, Urbana, IL;* <sup>2</sup>*University of Illinois at Chicago, Chicago, IL*
- ThP 389 **Rapid Identify Peptides in Biological Samples using Antibody Conjugated Beads and Mass Spectrometry;** Rong-Ming Lyu; [Jaw-Kang Chang](#); *Phoenix Pharmaceuticals, Burlingame, CA*
- ThP 390 **Peptidomic Investigation of the Rat Dorsal Root Ganglia Secretome;** [Emily Tillmaand](#); Ning Yang; Callie Croushore; Elena Romanova; Stanislav Rubakhin; Jonathan Sweedler; *University of Illinois at Urbana-Champaign, Urbana, IL*
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- ThP 393 **Diagonal Chromatography with High Density Sampling, Computational Reconstruction and Targeted Validation;** [Lasse Falkenby](#); Martin R. Larsen; *University of Southern Denmark, Odense, Denmark*
- ThP 394 **Optimization of 2D- chromatographic Conditions for Deeper Proteome Coverage and Higher Duty Cycle in MudPIT Proteome Experiments;** [Ramsunder Iyer](#)<sup>1,2</sup>; Richard Giannone<sup>1</sup>; Robert Hettich<sup>1</sup>; <sup>1</sup>*Oak Ridge National Laboratory, Oak Ridge, TN;* <sup>2</sup>*University of Tennessee, Knoxville, TN*
- ThP 395 **Normal Phase Separation of Peptides for Proteomic Experiments;** [Andreas Fichtenbaum](#)<sup>1</sup>; Rainer Schmid<sup>1</sup>; Goran Mitulovic<sup>2</sup>; <sup>1</sup>*Medical University of Vienna, Vienna, Austria;* <sup>2</sup>*Medical University of Vienna, KIMCL, Vienna, N/A*
- ThP 396 **Online Hydrophobic Interaction Chromatography Mass Spectrometry for Top-down Proteomics;** [Bifan Chen](#)<sup>1</sup>; Santosh Valeja<sup>1</sup>; Ying Peng<sup>1</sup>; Lichen Xiu<sup>1</sup>; Andrew Alpert<sup>1,2</sup>; Ying Ge<sup>1</sup>; <sup>1</sup>*University of Wisconsin-Madison, Madison, WI;* <sup>2</sup>*PolyLC Inc., Columbia, MD*
- ThP 397 **Automated Switching between nanoLC Workflows: Sample Trapping and Direct Injection;** [Alexander Boychenko](#); Christoph Hollnagel; Remco Swart; *Thermo Fisher Scientific, Germering, Germany*
- ThP 398 **2D-LCMS Analysis of Intact Glycoproteins – A Feasibility Study of Running Ion Exchange Chromatography and Fast Reverse Phase LCMS;** [Lisa Zang](#); Yanan Yang; Ning Tang; *Agilent Technologies, Inc, Santa Clara, CA*
- ThP 399 **Prediction of Peptide Retention Times in Hydrophilic Interaction Liquid Chromatography (HILIC) Based on Amino Acid Composition;** [Majors Badgett](#)<sup>1</sup>; Barry Boyes<sup>2</sup>; Ron Orlando<sup>1</sup>; <sup>1</sup>*University of Georgia, Athens, GA;* <sup>2</sup>*Advanced Materials Technology, Wilmington, DE*
- ThP 400 **Evaluating the Utility of Micro-flow Chromatography for Peptide MRM Assays;** [Lisa Wolfe](#); Carolina Mehaffy; Jay Kirkwood; Jessica Prenni; *Colorado State University, Fort Collins, CO*
- ThP 401 **Dual Channel Microflow LC-MS: Investigations of High Sensitivity and High Throughput;** [David Neyer](#); Remco van Soest; Khaled Mriziq; *SCIEX, Redwood City, CA*
- ThP 402 **Intact Protein Separation and Quantification in Biological Fluids using HPLC and Triple Quadrupole Mass Spectrometry;** [Evelyn Wang](#)<sup>1</sup>; Dananjaya Kalu Appulage<sup>1</sup>; Frances Carroll<sup>2</sup>; Kevin Schug<sup>1</sup>; <sup>1</sup>*University of Texas at Arlington, Arlington, TX;* <sup>2</sup>*Restek Corporation, Bellefonte, PA*
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- ThP 404 **Agricultural Applications of SFC-MS;** [Jeffrie Godbey](#)<sup>1</sup>; Tony Brand<sup>2</sup>; Mary Evenson<sup>1</sup>; Jeffrey Gilbert<sup>1</sup>; Mingming Ma<sup>1</sup>; Esther Rodriguez-Rosas<sup>1</sup>; Jennifer Vananda<sup>2</sup>; <sup>1</sup>*Dow AgroSciences, Indianapolis, IN;* <sup>2</sup>*Agilent Technologies, Santa Clara, CA*
- ThP 405 **Continuous Post-Column Standard Infusion for Calibration and Correction of UHPLC-QqQ-LC Data;** [Lin Wang](#); Qian Wu; Stanislav Rubakhin; Jonathan Sweedler; *University of Illinois at Urbana-Champaign, Urbana, IL*
- ThP 406 **Analysis of Leucine and Metabolites  $\beta$ -hydroxy- $\beta$ -methylbutyric Acid,  $\alpha$ -ketoisocaproic Acid, and  $\alpha$ -hydroxyisocaproic Acid in Human Breast Milk by Liquid Chromatography-Mass Spectrometry;** [Stefan Ehling](#); Todime Reddy; *Abbott Nutrition, Columbus, OH*
- ThP 407 **Optimization and Evaluation of Nanoflow UHPLC-MS for Chemical Isotope Labelling Metabolomics;** [Jaspaul Tatlay](#); Zhendong Li; Liang Li; *University of Alberta, Edmonton, Canada*
- ThP 408 **Quantitative Measurement of Urinary Diamines as Biomarkers of Exposure to Diisocyanates using UPLC-ESI-MS/MS;** [Deepak Bhandari](#)<sup>1</sup>; Udeni Alwis<sup>1</sup>; Hongzhu Liao<sup>2</sup>; Yu (Emily) Qiu<sup>1</sup>; Benjamin Blount<sup>1</sup>; <sup>1</sup>*Center for Disease Control and Prevention, Atlanta, GA;* <sup>2</sup>*University of Texas at Arlington, Arlington, TX*
- ThP 409 **High Throughput Simultaneous Analysis of 39 Amino Acids in Various Foods without Derivatization using LC-MS/MS;** [Manabu Yukiya](#)<sup>1</sup>; Keiko Matsumoto<sup>1</sup>; Jun Watanabe<sup>1</sup>; Itaru Yazawa<sup>2</sup>; <sup>1</sup>*Shimadzu Corporation, Kyoto, Japan;* <sup>2</sup>*Imtakt Corporation, Kyoto, Japan*
- ThP 410 **LCMS of Glyco-Conjugate Oligomers: Separation and Characterization;** Bela Reiz; Vijaya Ganesh; David Bundle; [Randy Whittall](#); *University of Alberta, Edmonton, Canada*
- ThP 411 **Automated LC-MS Method Development for Small Molecule Separation using Different Reversed Phase Column Chemistries;** [Dananjaya Kalu Appulage](#)<sup>1</sup>; Evelyn Wang<sup>1</sup>; Frances Carroll<sup>2</sup>; Kevin Schug<sup>1</sup>; <sup>1</sup>*University of Texas at Arlington, Arlington, TX;* <sup>2</sup>*Restek Corporation, Bellefonte, PA*



- ThP 412 **Ultra High Performance Liquid Chromatography-Triple Quadrupole Mass Spectrometry Detection of Hydroxy Acids in Complex Mixtures from Prebiotic Simulation Experiments**; Eric Parker<sup>1</sup>; Jeffrey Bada<sup>2</sup>; Facundo Fernandez<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, U.S.A.; <sup>2</sup>Scripps Institution of Oceanography, UC San Diego, La Jolla, CA
- ThP 413 **An Optimized Protocol for the Use of DMSO Cosolvent With Q Exactive Mass Spectrometer to Improve Peptide Sequencing Depth Significantly**; Zhuo Chen; Arthur Salomon; Brown University, Providence, RI
- ThP 414 **High Sensitive LC/MS Analysis of High Polar Compounds using Polymer-Based Amino Column**; Junji Sasuga<sup>1</sup>; Ronald Benson<sup>2</sup>; Jun Watanabe<sup>3</sup>; <sup>1</sup>Showa Denko K.K., Kawasaki, Japan; <sup>2</sup>Showa Denko America, Inc., New York, NY; <sup>3</sup>Shimadzu Corporation, Kyoto, Japan
- ThP 415 **Capillary Liquid Chromatography Mass Spectrometry Analysis of Trimethylamine and Trimethylamine N-oxide and Creatinine in Mouse Urine**; Sunil Veeravalli<sup>1</sup>; Kersti Karu<sup>2</sup>; Elizabeth H Shepherd<sup>1</sup>; <sup>1</sup>Department of Structural and Molecular Biology, UCL, London, UK; <sup>2</sup>Department of Chemistry, Christopher Ignold Build, UCL, London, UK
- ThP 416 **Effect of Mobile Phase Solvents and Additives on LC-MS Response of PD0332991 by Selected Ion Monitoring and Tandem Mass Spectrometry**; Subhra Bhattacharya; Stephen C. Roemer; Thermo Fisher Scientific, Fair Lawn, NJ
- ThP 417 **On-line LC×LC-MS/MS: a Powerful Unified Separation-science Tool**; Paola Donato<sup>1</sup>; Francesca Rigano<sup>1</sup>; Ambrogina Albergamo<sup>1</sup>; Francesco Cacciola<sup>1</sup>; Marco Beccaria<sup>1</sup>; Paola Dugo<sup>1,2</sup>; Luigi Mondello<sup>1,3</sup>; <sup>1</sup>University of Messina, Messina, Italy; <sup>2</sup>University Campus Bio-Medico of Rome, Rome, Italy; <sup>3</sup>Chromaleont s.r.l., c/o University of Messina, Messina, Italy
- ThP 418 **High Throughput Regulatory Analysis of Phthalates and Parabens in Cosmetics and Personal Care Products, using UPLC with Mass Detection**; Jane Cooper; Oliver Burt; Waters Corporation, Wilmslow, UK
- ThP 419 **Development of a Metabolome Analysis Method for Intracellular Central Metabolites by LC-MS/MS without using Ion-Pairing Reagents**; Tomokazu Shirai<sup>1</sup>; Tsuyoshi Nakanishi<sup>2</sup>; Masaki Yamada<sup>2</sup>; Akihiko Kondo<sup>3</sup>; <sup>1</sup>RIKEN, Yokohama-Shi, Japan; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan; <sup>3</sup>Kobe University, Kobe, Japan
- ThP 420 **Intact Amino Acid Isomers Separation using a Novel Specialized Column by LC-MS without Derivatization**; Iitaru Yazawa; Hiroshi Tachikawa; Imtakt Corporation, Kyoto, Japan
- ThP 421 **Fast and Straightforward Approaches for the LC-MS and LC-MS/MS Analysis of Food and Pharma Samples**; Stephan Altmaier<sup>1</sup>; David Lentz<sup>2</sup>; <sup>1</sup>Merck Millipore, Merck KGaA, Darmstadt, Germany; <sup>2</sup>EMD Millipore, Billerica, MA
- ThP 422 **The Dried Blood Spots Analysis of Endogenous Levels of β-hydroxy-β-methylbutyric Acid in Human Blood using Dual Stable Labeled Isotopic Standards**; Carl Noren; Stefan Ehling; Nicholas Cellar; Todime Reddy; Abbott Nutrition, Columbus, OH
- ThP 423 **Effect of Packing Material and Hardware of LC Column on Sensitive Analysis of Chelating Compounds using LC/MS/MS**; Koji Suzuki; Chiaki Aoyama; Yukinori Konno; Kosuke Osaka; Jun-ichi Hashimoto; Yukio Otsuka; Atsushi Sato; GL Sciences Inc., Shinjuku-Ku, Japan
- ThP 424 **A New Alternative Method for Impurity Profiling of Olmesartan Medoxomil using LC-MS/MS**; Anita Piper; Stephan Altmaier; Merck Millipore, Merck KGaA, Darmstadt, Germany
- ThP 425 **A Proposed USP/EP Method for the Determination of Spectinomycin Impurities by LC-MS**; Carmen T. Santasania<sup>1</sup>; Andy Ommen<sup>2</sup>; Nicolas J. Hauser<sup>2</sup>; <sup>1</sup>Supelco/Sigma-Aldrich, Bellefonte, PA; <sup>2</sup>RTC/Sigma-Aldrich, Laramie, WY
- ThP 426 **Characterization of Products Formed by Forced Degradation of Etodolac using LC/MS/MS**; Shailesh Damale<sup>1</sup>; Deepti Bhandarkar<sup>1</sup>; Shruti Raju<sup>1</sup>; Shailendra Rane<sup>1</sup>; Rashi Kochhar<sup>1</sup>; Ajit Datar<sup>1</sup>; Pratap Rasam<sup>1</sup>; Jitendra Kelkar<sup>1</sup>; Divya Saxena<sup>2</sup>; <sup>1</sup>Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India; <sup>2</sup>G.N.I.R.D., G.N. Khalsa College, Mumbai, India
- ThP 427 **A "High Throughput" Picogram Sensitivity LC-MS/MS Method for the Quantitation of Rivastigmine in Human Plasma**; Yuzhu Xue; Yuan-Shek Chen; QPS, LLC, Newark, DE
- ThP 428 **Phosphorylation of Organic Compounds with the Schreibersite Analog Fe<sub>3</sub>P**; Mike Mojica<sup>1</sup>; Maheen Gull<sup>2</sup>; David Gaul<sup>1</sup>; Charles Liotta<sup>1</sup>; Matthew Pasek<sup>2</sup>; Facundo Fernandez<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, Ga; <sup>2</sup>University of South Florida, Tampa, FL
- ThP 429 **Assessment of the Selectivity and Plasma Metabolome Coverage of Complementary HILIC Stationary Phases**; Stefanie Wernisch<sup>1</sup>; Li Zhang<sup>2</sup>; Subramaniam Pennathur<sup>1,2</sup>; <sup>1</sup>Dept. of Internal Medicine, University of Michigan, Ann Arbor, MI; <sup>2</sup>Metabolomics Resource Core, University of Michigan, Ann Arbor, MI
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- ThP 431 **XLH: A Tool to Harmonize and Integrate Output from Multi-Threaded XL-MS Workflows and Multiple, Parallel XL-MS Crosslink Detection Programs**; Paul Gershon; UC-Irvine, Irvine, CA
- ThP 432 **Confident Identification of Chemical Crosslinks in Nonspecifically-Digested LC-MS/MS Samples by Locus-Centric Aggregate Scoring**; Mark Adamo<sup>1</sup>; Andrew Grasseti<sup>2</sup>; Scott Gerber<sup>2</sup>; <sup>1</sup>Norris Cotton Cancer Center, Lebanon, NH; <sup>2</sup>Geisel School of Medicine, Lebanon, NH
- ThP 433 **Identification via Shotgun Mass Spectrometry of Unlabelled Chemical Crosslinks in Protein Complexes, using XCorr, Exact p-value calibration, and Parsimonious Search**; J. Jeffry Howbert; William Noble; University of Washington, Seattle, WA
- ThP 434 **LC-MS/MS Peptide Mapping with de novo Sequencing for Cross-Linking Peptide Analysis**; Baozhen Shan; Lei Xin; Bioinformatics Solutions Inc., Waterloo, Canada
- ThP 435 **A Novel Statistical Learning Model for Mass Spectrometric Identifications of Cross-Linked Peptides**; Chao Ji; James P. Reilly; Predrag Radivojac; Haixu Tang; Indiana University, Bloomington, IN
- ThP 436 **Kojak: Efficient Analysis of Chemically Cross-Linked Protein Complexes**; Michael R. Hoopmann<sup>1</sup>; Alex Zelter<sup>2</sup>; Richard S. Johnson<sup>2</sup>; Michael Riffle<sup>2</sup>; Michael J. Maccoss<sup>2</sup>; Trisha N. Davis<sup>2</sup>; Robert L. Moritz<sup>1</sup>; <sup>1</sup>Institute for Systems Biology, Seattle, WA; <sup>2</sup>University of Washington, Seattle, WA
- ThP 437 **SIM-XL: A Powerful and User-Friendly Tool for Peptide Cross-Linking Analysis**; Diogo Borges Lima<sup>1</sup>; Tatiani B de Lima<sup>2</sup>; Tiago S Balbuena<sup>3</sup>; Ana Gisele C. Neves-Ferreira<sup>4</sup>; Valmir C Barbosa<sup>5</sup>; Fabio C Gozzo<sup>2</sup>; Paulo C Carvalho<sup>1</sup>; <sup>1</sup>Lab Proteomics Protein Engineering - ICC - Fiocruz, Curitiba, PR; <sup>2</sup>Dalton Mass Spectrometry Laboratory - Unicamp, Campinas, SP; <sup>3</sup>College of Agricultural and Veterinary Sciences, Jaboticabal, SP; <sup>4</sup>Laboratory of Toxinology - IOC - Fiocruz, Rio de Janeiro, RJ; <sup>5</sup>Systems Engineering and Computer Science Program, Rio de Janeiro, RJ

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- ThP 438 **ProMex: A New Feature Extraction Algorithm for Top-down Mass Spectrometry Based on Summed Spectra;** Jungkap Park; Paul D. Piehowski; Christopher S. Wilkins; Anil K. Shukla; Yufeng Shen; Samuel H. Payne; Richard D. Smith; Sangtae Kim; *PNNL, Richland, WA*
- ThP 439 **A Facile Synthetic Route Towards A Novel Isobaric Tag Architecture For Increased Multiplexing and Improved Complement Reporter Ion Formation;** Craig Braun<sup>1</sup>; Martin Wühr<sup>1</sup>; Brian Erickson<sup>1</sup>; Gregory Bird<sup>2</sup>; Steven Gygi<sup>1</sup>; Wilhelm Haas<sup>1</sup>; <sup>1</sup>*Harvard Medical School, Boston, MA*; <sup>2</sup>*Dana Farber Cancer Institute, Boston, MA*
- ThP 440 **High Quality Top-Down Proteomics Analysis Using R;** Christian Heckendorf<sup>1</sup>; Roger Theberge<sup>2</sup>; Jean Spencer<sup>1</sup>; Catherine E. Costello<sup>1</sup>; Mark E. Mccomb<sup>1</sup>; <sup>1</sup>*Boston University School of Medicine, Boston, MA*; <sup>2</sup>*Boston University School, Boston, MA*
- ThP 441 **New Functionality for the Trans-Proteomic Pipeline: Tools for the Analysis of Proteomics Data;** Luis Mendoza<sup>1</sup>; David Shteynberg<sup>1</sup>; Joseph Slagel<sup>1</sup>; Michael R. Hoopmann<sup>1</sup>; Henry Lam<sup>2</sup>; Jimmy K Eng<sup>3</sup>; Eric Deutsch<sup>1</sup>; Robert L Moritz<sup>1</sup>; <sup>1</sup>*Institute For Systems Biology, Seattle, WA*; <sup>2</sup>*Hong Kong University of Science and Technology, Hong Kong, China*; <sup>3</sup>*University of Washington, Seattle, WA*
- ThP 442 **Morpheus Spectral Counter: A Computational Tool for Label-Free Quantitative Mass Spectrometry using the Morpheus Mass Spectrometry Search Engine;** David C. Gemperline; Mark Scaff; Richard D Vierstra; *UW Madison, Madison, Wisconsin*
- ThP 443 **A Common Data Analysis Pipeline for the Clinical Proteomics Tumor Analysis Consortium (CPTAC);** Paul Rudnick<sup>1</sup>; Sanford Markey<sup>2</sup>; Jeri Roth<sup>2</sup>; Yuri Mirokhin<sup>2</sup>; Nathan Edwards<sup>3</sup>; Stephen Stein<sup>2</sup>; <sup>1</sup>*Spectragen Informatics, Rockville, MD*; <sup>2</sup>*NIST, Gaithersburg, MD*; <sup>3</sup>*Georgetown University Medical Center, Washington, DC*
- ThP 444 **Development of Sample-Specific Spectral Libraries to Increase Coverage of Mass Spectrometry-Based Proteomic Data for Samples of Limited Available Amounts;** Krishan Kumar<sup>1</sup>; Himanshu Grover<sup>2</sup>; Simion Kreimer<sup>1</sup>; David Fenyó<sup>2</sup>; Alexander R. Ivanov<sup>1</sup>; Barry L. Karger<sup>1</sup>; <sup>1</sup>*Barnett Inst., Northeastern University, Boston, MA*; <sup>2</sup>*New York University, New York, NY*
- ThP 445 **A Novel Approach for Relative Protein Quantitation by Spectral Counting;** Guoan Zhang; Jingjing Deng; Thomas Neubert; *Skirball Institute, NYUMC, New York, NY*
- ThP 446 **MASH Suite Pro: A Comprehensive Tool for Top-down Proteomics;** Wenxuan Cai<sup>1</sup>; Huseyin Guner<sup>1</sup>; Santosh Valeja<sup>1</sup>; Ying Peng<sup>1</sup>; Xiaowen Liu<sup>2</sup>; Ying Ge<sup>1</sup>; <sup>1</sup>*UW-Madison, Madison, WI*; <sup>2</sup>*Indiana University-Purdue University, Indianapolis, IN*
- ThP 447 **De novo Sequencing of E.coli Lysate Using a Single Series of Fragment Ions via Chromophore Tagging and 351 nm UVPD;** Scott Robotham<sup>1</sup>; Andrew Horton<sup>1</sup>; Joe Cannon<sup>2</sup>; Edward Marcotte<sup>1</sup>; Jennifer Brodbelt<sup>1</sup>; <sup>1</sup>*University of Texas at Austin, Austin, TX*; <sup>2</sup>*Tufts University, Medford, MA*
- ThP 448 **Combination Optimization of Search Engines and Post-Processing Approaches to Maximize Peptide/Protein Identification for Analyzing High Accuracy Mass Spectra;** Chengjian Tu<sup>1</sup>; Quanhu Sheng<sup>2</sup>; Danjun Ma<sup>3</sup>; Xiaomeng Shen<sup>1</sup>; xue Wang<sup>1</sup>; Yu Shyr<sup>2</sup>; Zhengping Yi<sup>3</sup>; Jun Qu<sup>1</sup>; <sup>1</sup>*University at Buffalo, Buffalo, NY*; <sup>2</sup>*Vanderbilt University School of Medicine, Nashville, TN*; <sup>3</sup>*Wayne State University, Clawson, MI*
- ThP 449 **A Novel Ion-current-based MS1 Strategy with Hybrid High-field Orbitrap Enables Large-Scale, Accurate, Extensive Proteomic Quantification with Extremely Low Missing Data;** Xiaomeng Shen<sup>1,3</sup>; Jun Li<sup>2,3</sup>; Chengjian Tu<sup>2,3</sup>; Shichen Shen<sup>1,3</sup>; Xue Wang<sup>4</sup>; Jun Qu<sup>2,3</sup>; <sup>1</sup>*Dept. of Biochemistry at SUNY at Buffalo, Buffalo, NY*; <sup>2</sup>*Dept. of Pharmaceutical Sci. at SUNY at Buffalo, Buffalo, NY*; <sup>3</sup>*Center of Excellence in Bioinformatics&Life Sci., Buffalo, NY*; <sup>4</sup>*Rosewell Park Cancer Institute, Buffalo, NY*
- ThP 450 **TopPIC: A Software Tool for Top-Down Mass Spectrometry-Based Proteoform Identification and Characterization;** Qiang Kou<sup>1</sup>; Likun Xun<sup>1</sup>; Xiaowen Liu<sup>1,2</sup>; <sup>1</sup>*Indiana University Purdue University Indianapolis, Indianapolis, IN*; <sup>2</sup>*Indiana University School of Medicine, Indianapolis, IN*
- ThP 451 **Large Scale Quantitation of Stable Isotope Labeled Proteomes Using Retention and Drift Time Profiling;** Andrew Collins<sup>1</sup>; Antony McCabe<sup>1</sup>; Ian Morns<sup>3</sup>; Johannes PC Vissers<sup>2</sup>; Andrew R Jones<sup>1</sup>; <sup>1</sup>*Institute of Integrative Biology, University of Liverpool, UK*; <sup>2</sup>*Waters Corporation, Manchester, UK*; <sup>3</sup>*Nonlinear Dynamics Limited, Newcastle upon Tyne, UK*
- ThP 452 **New Method for Evaluating the Protein Significance in the Label-free Quantification;** Lei Xin; Baozhen Shan; *Bioinformatics Solutions Inc., Waterloo, Canada*
- ThP 453 **Deep, single shot human cell line protein profiling using DIA and Spectronaut on a Q Exactive HF;** Roland Bruderer<sup>1</sup>; Yue Xuan<sup>2</sup>; Oliver Bernhardt<sup>1</sup>; Tejas Gandhi<sup>1</sup>; Lukas Reiter<sup>1</sup>; <sup>1</sup>*Biognosys AG, Schlieren, Switzerland*; <sup>2</sup>*ThermoFisherScientific, Bremen, Germany*

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- ThP 455 **A Novel Analytical-Informatics Platform Reveals the Hidden Tryptic Peptidome and Improves Multi-omic Applications;** Candace R. Guerrero<sup>1</sup>; Pratik Jagtap<sup>2</sup>; James Johnson<sup>1</sup>; Getiria Onsongo<sup>1</sup>; Trevor Wennblom<sup>1</sup>; Jae-Woong Chang<sup>1</sup>; Susan K. Van Riper<sup>2</sup>; Todd Markowski<sup>2</sup>; Jeongsik Yong<sup>1</sup>; Timothy J. Griffin<sup>1</sup>; <sup>1</sup>*University of Minnesota, Minneapolis, MN*; <sup>2</sup>*Center for Mass Spectrometry and Proteomics, UMN, St. Paul, MN*
- ThP 456 **Comparative Study of Predicted Highly Expressed Genes with the Proteins Detected from Clostridium thermocellum Grown on Switchgrass;** Suresh Poudel<sup>1,2</sup>; Richard Giannone<sup>1</sup>; Intawat Nookaew<sup>1</sup>; David Ussery<sup>1</sup>; Robert Hettich<sup>1</sup>; <sup>1</sup>*Oak Ridge National Laboratory, Oak Ridge, TN*; <sup>2</sup>*University of Tennessee, Knoxville, TN*
- ThP 457 **Peptide Centric Functional Enrichment for Complex Proteomics Datasets;** Vikram Mitra<sup>1</sup>; David Britton<sup>1</sup>; Vadim Farztdinov<sup>1</sup>; Alberto Quaglia<sup>2</sup>; Yoh Zen<sup>3</sup>; Claire Russell<sup>1</sup>; Malcolm Ward<sup>1</sup>; Emma Lahert<sup>1</sup>; Ian Pike<sup>1</sup>; <sup>1</sup>*Proteome Sciences plc, Cobham, UK*; <sup>2</sup>*Institute of Liver Studies, King's College Hospital, London, UK*; <sup>3</sup>*University Graduate School of Medicine, Kobe, JP*
- ThP 458 **Antibody Identification from a Polyclonal Mixture using Immunoproteogenomics;** Stefano Bonissone<sup>1</sup>; Yana Safonova<sup>2,3</sup>; Eugene Kurpilyansky<sup>2,3</sup>; Ekaterina Starostina<sup>2</sup>; Alla Lapidus<sup>2,3</sup>; Wendy Sandoval<sup>4</sup>; Jennie Lill<sup>4</sup>; Pavel Pevzner<sup>1</sup>; <sup>1</sup>*University of California at San Diego, San Diego, CA*; <sup>2</sup>*St. Petersburg Academic University, St Petersburg, Russia*; <sup>3</sup>*St. Petersburg State University, St. Petersburg, Russia*; <sup>4</sup>*Genentech, South San Francisco, CA*
- ThP 459 **Glioblastoma Multiforme Subtype Classification: Integrated Analysis of Protein and Gene Expression Data;** Durairaj Renu<sup>1</sup>; Vadiraja Bhat<sup>3</sup>; Mona Al-Gizawiy<sup>2</sup>; Carolina B. Livi<sup>3</sup>; Stephen Madden<sup>3</sup>; Christine A. Miller<sup>3</sup>; Michael Rosenberg<sup>3</sup>; Kathleen Schmainda<sup>2</sup>; Prateek Singh<sup>1</sup>; Pramila Tata<sup>1</sup>; Shama P. Mirza<sup>2</sup>; <sup>1</sup>*Strand Life Sciences, Bangalore, India*; <sup>2</sup>*Medical College of Wisconsin, Milwaukee, WI*; <sup>3</sup>*Agilent Technologies, Inc., Santa Clara, CA*





- ThP 460 **Comprehensive Database Search Strategy for Proteogenomics**; Harsha P. Gunawardena<sup>1</sup>; John Wrobel<sup>1</sup>; Jonathon O'Brien<sup>1</sup>; Ling Xie<sup>1</sup>; Kelly Ruggles<sup>2</sup>; David Fenyo<sup>2</sup>; Sherri Davies<sup>3</sup>; Li Ding<sup>3</sup>; Reid Townsend<sup>3</sup>; Matthew Ellis<sup>4</sup>; Bhajat F. Qaqish<sup>1</sup>; Xian Chen<sup>1</sup>; <sup>1</sup>University of North Carolina at Chapel Hill, Chapel Hill, NC; <sup>2</sup>NYU Langone Medical Center, New York, NY; <sup>3</sup>Washington University School of Medicine, St. Louis, Missouri; <sup>4</sup>Baylor College of Medicine, Houston, TX
- ThP 461 **Mitochondria-driven Cancer Pathways in Triple Negative Breast Cancer**; Jun H. Park<sup>1</sup>; Vadiraja B. Bhat<sup>2</sup>; Santhosh Kumar<sup>1</sup>; Sajna A. Vithayathil<sup>1</sup>; Nagireddy Putluri<sup>1</sup>; Efosini Tsouko<sup>1</sup>; Taraka R. Donti<sup>1</sup>; Daniel E. Frigo<sup>1</sup>; Chad J. Creighton<sup>1</sup>; Michael T. Lewis<sup>1</sup>; Arun Sreekumar<sup>1</sup>; Lee-Jun Wong<sup>1</sup>; Benny A. Kaiparettu<sup>1</sup>; <sup>1</sup>Baylor College of Medicine, Houston, TX; <sup>2</sup>Agilent Technologies, Wilmington, DE
- ThP 462 **Proteomic Analysis Augments Lipidomic and Metabolomic Understanding of Hepatic Changes on High Fat Diets**; Devin L. Drew<sup>1</sup>; Daniela M. Schlatter<sup>2</sup>; Michelle A. Puchowicz<sup>2</sup>; Mark R. Chance<sup>2</sup>; David A. Peake<sup>1</sup>; Junhua Wang<sup>1</sup>; Andreas F. Huhmer<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Case Western Reserve University, Cleveland, OH
- ThP 463 **Statistical and Pathway Analysis of Protein Data**; Stephen Madden<sup>1</sup>; Joseph C. Roark<sup>1</sup>; Vadiraja Bhat<sup>1</sup>; Carolina B. Livi<sup>1</sup>; Christine A. Miller<sup>1</sup>; Mona Al-Gizawiy<sup>2</sup>; Kathleen Schmaida<sup>2</sup>; Shama P. Mirza<sup>2</sup>; <sup>1</sup>Agilent Technologies, Inc., Santa Clara, CA; <sup>2</sup>Medical College of Wisconsin, Milwaukee, WI
- ThP 464 **Harnessing Public Data Repositories for Metaproteomics**; Natalie Castellana; Digital Proteomics, LLC., San Diego, CA
- ThP 465 **Multi-Omics Analysis of Estradiol and Propyl Pyrazole Triol Treatment Effects in MCF7 Cells as Part of the Human Toxome Project**; Vadiraja B. Bhat<sup>2</sup>; Carolina B. Livi<sup>2</sup>; Christine Miller<sup>2</sup>; Rick A. Fasani<sup>2</sup>; Michael Rosenberg<sup>2</sup>; Renxiang Chen<sup>3</sup>; Henghong Li<sup>3</sup>; Albert J. Fornace Jr.<sup>3</sup>; James D. Yager<sup>1</sup>; Shelly Odwin-DaCosta<sup>1</sup>; Kim Boekelheide<sup>4</sup>; Marguerite M Vantangoli<sup>4</sup>; Melvin E. Andersen<sup>4</sup>; Patrick D McMullen<sup>4</sup>; Salil Pendse<sup>4</sup>; Alex Maertens<sup>1</sup>; Thomas Luechtelfeld<sup>1</sup>; Andre Kleensang<sup>1</sup>; Mounir Bouhifd<sup>1</sup>; Thomas Hartung<sup>1</sup>; <sup>1</sup>Johns Hopkins University, Baltimore, MD; <sup>2</sup>Agilent Technologies, Santa Clara, CA; <sup>3</sup>Georgetown University, Washington, DC; <sup>4</sup>Brown University, Providence, RI
- ThP 466 **Active Data Canvas: Web-Based Visual Analytic Tool to Link Data to Knowledge**; Joon-Yong Lee; Debjit Ray; Vladislav A. Petyuk; Richard D. Smith; Nick Cramer; Samuel H. Payne; Pacific Northwest National Laboratory, Richland, WA
- ThP 467 **Combining Ribosome Profiling and Proteomics to Discover Micropeptides, Translation Products from Small Open Reading Frames**; Volodimir Olexiouk; Jeroen Crappé; Steven Verbruggen; Wim Van Criekeing; Gerben Menschaert; Ghent University, Gent, Belgium
- ThP 468 **Automated Classification of Translated Genomic Elements Identified by Proteomics Informed by Transcriptomics**; Shyamasree Saha<sup>1</sup>; Jun Fan<sup>1</sup>; Vanessa Evans<sup>2</sup>; Gary Barker<sup>2</sup>; Kate Heesom<sup>2</sup>; David Matthews<sup>2</sup>; Conrad Bessant<sup>1</sup>; <sup>1</sup>Queen Mary, University of London, London, UK; <sup>2</sup>University of Bristol, Bristol, UK
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- ThP 469 **Prediction of Tertiary Structure of SalBIII Protein using Chemical Cross-Linking and Hydrogen/Deuterium Exchange (HDX) Coupled with Mass Spectrometry**; Hugo César Ramos De Jesus<sup>1</sup>; Gabriela D. Tormet Gonzalez<sup>1</sup>; Tiago S. Balbuena<sup>2</sup>; Luciana Gonzaga de Oliveira<sup>1</sup>; Fabio C Gozzo<sup>1</sup>; <sup>1</sup>UNICAMP, Campinas, Brazil; <sup>2</sup>UNESP, Jaboticabal, SP
- ThP 470 **Mapping Dynamic Interactions of a DNA Repair Enzyme with Its DNA Substrate by Site-Specific proTein-DNA UV Cross-Linking and Mass Spectrometry**; Fiona Flett; C. Logan Mackay; Heidrun Interthal; University of Edinburgh, Edinburgh, UK
- ThP 471 **Development of Electrochemical Mass Spectrometry for Probing Protein Three Dimensional Structures Using Isotope Labeled Cross-Linkers**; Qiuling Zheng; Hao Chen; Ohio University, Athens, OH
- ThP 472 **Monitoring of Human Haptoglobin-Hemoglobin Interaction Interface using Chemical Cross Linking and Hydrogen/Deuterium Exchange**; Zdenek Kukacka<sup>1, 2</sup>; Petr Man<sup>1, 2</sup>; Petr Novak<sup>1, 2</sup>; Petr Pompach<sup>1, 2</sup>; <sup>1</sup>Institute of Microbiology, Prague, Czech Republic; <sup>2</sup>Faculty of Sciences, Charles University in Prague, Prague, Czech Republic
- ThP 473 **Structural MS Analysis of Aldolase using a Dual Crosslinker Approach and the New CID-cleavable Crosslinker, MC4**; Lolita Piersimoni; Angela Walker; Hye Kyong Kweon; Hollis D Showalter; Philip C Andrews; University of Michigan, Ann Arbor, MI
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- ThP 476 **Quantitative Cross-Linking for Conformational Changes Analysis**; Luana Oliveira Dos Santos<sup>1</sup>; Marcelo Yudi Icimoto<sup>2</sup>; Alyne Maren Silva Barbosa<sup>2</sup>; Leandro Mantovani Castro<sup>3</sup>; Emer Suavinho Ferro<sup>3</sup>; Vitor Oliveira<sup>2</sup>; Fabio C. Gozzo<sup>1</sup>; <sup>1</sup>University of Campinas, Campinas, SP; <sup>2</sup>Federal University of São Paulo, São Paulo, SP; <sup>3</sup>University of São Paulo, São Paulo, SP
- ThP 477 **Mapping the Interaction between AGH Peptide and 14-3-3 Epsilon by Cross-Linking/MS and Molecular modelling**; Eliidiane G Da Silva<sup>1</sup>; Leandro M Castro<sup>2</sup>; Tiago S Balbuena<sup>3</sup>; Emer S Ferro<sup>2</sup>; Fabio C Gozzo<sup>1</sup>; IQ - University of Campinas, Campinas, Brazil; <sup>2</sup>University of São Paulo, São Paulo, Brazil; <sup>3</sup>UNESP, Jaboticabal, Brazil
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- ThP 480 **Chemical Crosslinking Coupled with Mass Spectrometry Enables Characterization of Protein Encounter Complexes**; Zhou Gong<sup>1</sup>; Yue-He Ding<sup>2</sup>; Da-Chuan Guo<sup>1</sup>; Wei-Ping Zhang<sup>3</sup>; Meng-Qiu Dong<sup>2</sup>; Chun Tang<sup>1</sup>; <sup>1</sup>Wuhan Institute of Physics and Mathematics, CAS, Wuhan, China; <sup>2</sup>National Institute of Biological Sciences,

- Beijing, Beijing, China; <sup>3</sup>Zhejiang University School of Medicine, Hangzhou, China
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- ThP 482 **Structural Analyses of the Oligomerization Mechanism of Amyloid  $\beta$  Peptides**; Ayumi Tanaka<sup>1</sup>; Shigeto Iwamoto<sup>1</sup>; Takashi Saito<sup>2</sup>; Hitomi Yamaguchi<sup>1</sup>; Sosuke Yoshinaga<sup>1</sup>; Yoshihiko Takinami<sup>3</sup>; Sawyen Ow<sup>4</sup>; Jouji Seta<sup>3</sup>; Toshiyuki Kohno<sup>5</sup>; Takaomi C. Saïdo<sup>2</sup>; Hiroaki Terasawa<sup>1</sup>; <sup>1</sup>Faculty of Life Sciences, Kumamoto University, Kumamoto, Japan; <sup>2</sup>RIKEN Brain Science Institute, Wako, Saitama, Japan; <sup>3</sup>Division of Application, Bruker Daltonics K. K., Yokohama, Japan; <sup>4</sup>Application, Bruker Sdn. Bhd., Selangor, Malaysia; <sup>5</sup>Kitasato University School of Medicine, Sagamihara, Japan
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- ThP 486 **Topology Analysis of Regulator Protein Complex by Chemical-Cross Mass Spectrometry**; Marcel Nakahira<sup>1</sup>; Nadia Rasheed<sup>1</sup>; Juliana Smetana<sup>1</sup>; David Sabatini<sup>3</sup>; Tiago Balbuena<sup>2</sup>; Fabio Gozzo<sup>1</sup>; <sup>1</sup>University of Campinas, Campinas, Brazil; <sup>2</sup>Universidade Estadual Paulista, Jaboticabal, Brazil; <sup>3</sup>Whitehead Institute for Biomedical Research, Cambridge, MA
- ThP 487 **Chemical Cross-Linking and Mass Spectrometry to Determine the Interaction Network of Protein Complexes**; Nha-Thi Nguyen-Huynh<sup>1</sup>; Grigory Sharov<sup>2</sup>; Clément Potel<sup>1</sup>; Pélagie Fichter<sup>2</sup>; Simon Trowitzsch<sup>3</sup>; Imre Berger<sup>3</sup>; Valérie Lamour<sup>2</sup>; Patrick Schultz<sup>2</sup>; Noëlle Potier<sup>1</sup>; Emmanuelle Leize-Wagner<sup>1</sup>; <sup>1</sup>LSMIS - UMR 7140 CNRS/Unistra, Strasbourg, France; <sup>2</sup>Integrated Structural Biology Department, IGBMC, Illkirch, France; <sup>3</sup>European Molecular Biology Laboratory (EMBL), Grenoble, France
- ThP 488 **Novel Crosslinking Chemistry for Protein Interaction Profiling and Bioconjugation**; Tristan McClure-Begley; Brady Worrell; Tao Gong; Christopher Ebmeier; Douglas Chapnick; Xuedong Liu; Christopher Bowman; William Old; University of Colorado, Boulder, CO
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- ThP 496 **Fast Photochemical Oxidation of Proteins (FPOP) for Quantitative Residue-level Analysis of Conformational Changes in Amyloid Beta Aggregation**; Ke Li; Ying Zhang; Don Rempel; Michael Gross; Washington University, St. Louis, MO
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- ThP 507 **Measurement of Cysteine -linked ADCs under Native Conditions using an Orbitrap Mass Analyzer**; Jing Li<sup>1</sup>; Shujun Yang<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, Shanghai, China; <sup>2</sup>NewBio Therapeutics, Inc, Shanghai, China
- ThP 508 **Analysis of non-Deglycosylated Antibody-Drug-Conjugates by TripleTOF® High Resolution Quadrupole-Time-Of-Flight Instrument and Effective Reconstruction Software**; Milla-Riina Neffling<sup>1</sup>; Bruno Genet<sup>2</sup>; David Bugnazet<sup>2</sup>; Eric Lacassie<sup>2</sup>; Justin Blethrow<sup>3</sup>; Eric Johansen<sup>3</sup>; <sup>1</sup>SCIEX, Warrington, UK; <sup>2</sup>Sanofi-Vitry Biologics SCP/Analytics, Vitry-Sur-Seine, France; <sup>3</sup>SCIEX, Red Wood Shores, CA
- ThP 509 **Rapid Method for Monitoring Monoclonal Antibody (mAb) Production in Biotechnological Processes using Quantitative MALDI-TOF-MS**; Robert Steinhoff<sup>1</sup>; Jasmin Krismer<sup>1</sup>; Martin Pabst<sup>2</sup>; Renato Zenobi<sup>1</sup>; <sup>1</sup>ETH Zurich, Zurich, Switzerland; <sup>2</sup>Polytherics, Cambridge, UK
- ThP 510 **Quantitative Analysis of Post Translation Modification of Protein Therapeutics at a Subunit Level by Spectral Deconvolution**; Ming Gu<sup>1</sup>; Kadir Ilker Sen<sup>2</sup>; Yongdong Wang<sup>1</sup>; Darryl Davis<sup>2</sup>; <sup>1</sup>Cerno Bioscience, Norwalk, CT; <sup>2</sup>Janssen Pharmaceutical Companies of Johnson & John, Springhouse, PA
- ThP 511 **High Sensitivity Native Mass Spectrometry Characterization of Antibody Fluorescent Conjugates (AFC)**; Caroline S. Chu<sup>1</sup>; Gregory Staples<sup>1</sup>; Andy Gieschen<sup>2</sup>; Ning Tang<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>Agilent Technologies, La Jolla, CA
- ThP 512 **Combining Top Down and Bottom Up MALDI TOF/TOF Data in the de novo Sequencing of Monoclonal Antibodies**; Andy Mahan<sup>1</sup>; Yazan Jmeian<sup>2</sup>; Darryl Davis<sup>1</sup>; <sup>1</sup>Johnson and Johnson, Spring House, PA; <sup>2</sup>Janssen Research & Development, Radnor, PA
- ThP 513 **Application of Capillary Electrophoresis Coupled to Quadrupole Time-of-Flight Mass Spectrometry for the Analysis of Immunoconjugates**; Suresh Babu CV<sup>1</sup>; Anne Basler<sup>2</sup>; Sina Bunzendahl<sup>2</sup>; Rainer Kneuer<sup>2</sup>; <sup>1</sup>Agilent Technologies, Bangalore, India; <sup>2</sup>Novartis Institutes for Biomed. Research, Basel, Switzerland
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- ThP 515 **Mass Spectrometric Investigation of Maleimide Linker Hydrolysis in Antibody-drug Conjugates**; Ling Xu<sup>1</sup>; Laura Packer<sup>1</sup>; Yue Zhang<sup>2</sup>; Shaoxia Yu<sup>1</sup>; Jing-Tao Wu<sup>1</sup>; Mark Qian<sup>1</sup>; <sup>1</sup>Takeda Pharmaceutical International Inc., Cambridge, MA; <sup>2</sup>BioAnalytix Inc, Cambridge, MA
- ThP 516 **Collision Induced Unfolding of Intact Antibodies, Biotherapeutics and Biosimilars: Rapid Characterization of Disulfide Bonding Patterns and Structures**; Yuwei Tian<sup>1</sup>; Linjie Han<sup>1</sup>; Adam Buckner<sup>1</sup>; Brandon Ruotolo<sup>1</sup>; Department of Chemistry, University of Michigan, Ann Arbor, MI
- ThP 517 **Peptide Mapping of Antibody Drug Conjugate using CE-ESI-MS**; Suresh Babu Cv; Ravindra Gudihal; Palaniswamy Meenakshi-Sundar M; Nilanjan Guha<sup>1</sup>; Sudha Rajagopalan<sup>1</sup>; Agilent Technologies, Bangalore, India
- ThP 518 **Analysis of Herceptin Oxidation Variants Using a Supermacro Porous Reverse Phase Column Coupled with an Orbitrap Mass Spectrometer**; Shanhua Lin<sup>1</sup>; Terry Zhang<sup>2</sup>; Hongxia (Jessica) Wang<sup>2</sup>; Jonathan L. Josephs<sup>2</sup>; Xiaodong Liu<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Sunnyvale, CA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- ThP 519 **Comprehensive Analysis of Intact Antibody Drug Conjugates using an Integrated Microfluidic HPLC-Chip MS Workflows**; Caroline S. Chu<sup>1</sup>; Andy Gieschen<sup>2</sup>; M Sundaram Palaniswamy<sup>3</sup>; Ning Tang<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>Agilent Technologies, La Jolla, CA; <sup>3</sup>Agilent Technologies Inc, Bangalore, India
- ThP 520 **Drug-to-Antibody Ratio Characterization of Antibody Drug Conjugate by Ion Mobility Mass Spectrometry**; Richard Huang<sup>1</sup>; David Passmore<sup>2</sup>; Vangipuram Rangan<sup>2</sup>; Shrikant Deshpande<sup>2</sup>; Adrienne Tymiak<sup>1</sup>; Guodong Chen<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb, Princeton, NJ; <sup>2</sup>Bristol-Myers Squibb, Redwood City, CA
- ThP 521 **Conformational Epitope Mapping of Angiotensin-2 (ANG-2) Specific Monoclonal Antibodies (mAb) by Partial Trypsin Digestion Followed by nanoLC-MRM**; Lei Wang<sup>1</sup>; Tetsuo Sekino<sup>2</sup>; Kenji Abe<sup>2</sup>; Mark Matijevic<sup>1</sup>; Jesse Chow<sup>1</sup>; Yoshiya Oda<sup>1</sup>; <sup>1</sup>Eisai Inc, Andover, MA; <sup>2</sup>EIDIA Co., Ltd., Inashiki, Japan
- ThP 522 **Overcoming Method-Related Challenges During Antibody Drug Conjugate Characterization by LC/MS**; Jacquelynn Smith<sup>1</sup>; Paul Brown<sup>1</sup>; Cecily Swabowski<sup>1</sup>; Jason Rouse<sup>2</sup>; James Carroll<sup>1</sup>; Olga Friese<sup>1</sup>; <sup>1</sup>Biotherapeutics Pharm. Sci., Pfizer Inc., St. Louis, MO; <sup>2</sup>Biotherapeutics Pharm. Sci., Pfizer Inc., Andover, MO
- ThP 523 **Characterization of Trisulfide Modifications of Recombinant Antibodies by Intact Mass Measurement and Non-Reduced Peptide Mapping**; Bianca Grünwalder<sup>1</sup>; Vincent Larraillet<sup>1</sup>; Oliver Popp<sup>1</sup>; Annette N.D. Scharf<sup>1</sup>; Maximiliane Hilger<sup>1</sup>; pRED, Roche Innovation Center, Penzberg, Germany
- ThP 524 **An Optimized Approach for the Sensitive Detection of Sequence Variants in Biotherapeutic Proteins**; Paul W. Brown<sup>1</sup>; James Carroll<sup>1</sup>; Jason Rouse<sup>2</sup>; <sup>1</sup>Pfizer, St. Louis, MO; <sup>2</sup>Pfizer, Andover, MA
- ThP 525 **Strategy for the Quantification of a Paclitaxel conjugated ADC (DAR  $\geq$  1) in Rat Plasma by LC-HRMS**; Jean-Nicholas Mess<sup>1</sup>; Fabio Garofolo<sup>1</sup>; Algorithm Pharma Inc., Laval, Canada
- ThP 526 **Separation and Characterization of Intact mAb Conjugate Charge Variants via Microfluidic CE-ESI with Online MS Analysis**; Erin A. Redman<sup>1</sup>; J. Scott Mellors<sup>2</sup>; J. Michael Ramsey<sup>1</sup>; <sup>1</sup>University of North Carolina at Chapel Hill, Chapel Hill, NC; <sup>2</sup>908 Devices Inc., Boston, MA
- ThP 527 **Quantitation of Cytotoxic Free Drug Released From an ADC into Conditioned Cell Culture Media**; Maria Christina Malinao<sup>1</sup>; Josh Snyder<sup>1</sup>; Julien Dugal-Tessier<sup>1</sup>; Christopher Kamball<sup>1</sup>; Min Wu<sup>1</sup>; Brian Mendelsohn<sup>1</sup>; Agensys, Inc., Santa Monica, CA
- ThP 528 **Analysis of Therapeutic Proteins Using Hydrophobic Interaction / Reversed-phase 2D-LC/MS with Multiple Heart-cutting**; Gregory Staples<sup>1</sup>; Hongfeng Yin<sup>1</sup>; Kevin Killeen<sup>1</sup>; Agilent Technologies, Santa Clara, CA
- ThP 529 **Use of Signature Ions with Accurate Mass and Collision Induced Dissociation to Unambiguously Assign Toxin Locations for Antibody Drug Conjugates**; Michael Bacica<sup>1</sup>; Aaron Wroblewski<sup>2</sup>; Jon Fitchett<sup>1</sup>; Bryan Jones<sup>1</sup>; <sup>1</sup>Lilly Biotech Center-San Diego, San Diego, CA; <sup>2</sup>LRL DCRT, Indianapolis, IN
- ThP 530 **A Comprehensive Quantitative Study of Monoclonal Antibody (mAb) by Q-TOF/MS and Ion Mobility Q-TOF/MS**; Ning Tang<sup>1</sup>; David L Wong<sup>1</sup>; Agilent Technologies, Santa Clara, CA

- ThP 531 **Rapid Detection of Deamidation in Monoclonal Antibodies using Ultrahigh-Resolution QTOF Mass Spectrometry**; [Wolfgang Jabs](#)<sup>1</sup>; Waltraud Evers<sup>1</sup>; Anja Wiechmann<sup>1</sup>; Jason Wood<sup>2</sup>; Guillaume Tremintin<sup>3</sup>; Detlev Suckau<sup>1</sup>; Keith Johnson<sup>4</sup>; Heather DeGruttola<sup>4</sup>; Lisa Marzilli<sup>4</sup>; Jason Rouse<sup>4</sup>; <sup>1</sup>*Bruker Daltonik GmbH, Bremen, Germany*; <sup>2</sup>*Bruker Daltonics Inc, Billerica, MA*; <sup>3</sup>*Bruker Daltonics Inc, Fremont, CA*; <sup>4</sup>*Pfizer Inc, Andover, MA*
- ThP 532 **Upstream Quality Control of Therapeutic Antibodies using Automated IdeS Digestion and Subunit Separation in Combination with Ultrahigh-Resolution QTOF Analysis**; Martin Hedström<sup>1</sup>; Fredrik Olsson<sup>2</sup>; Dag Erlandsson<sup>1</sup>; Anja Wiechmann<sup>3</sup>; Catherine Evans<sup>4</sup>; Guillaume Tremintin<sup>5</sup>; Jason Wood<sup>6</sup>; Detlev Suckau<sup>3</sup>; Wolfgang Jabs<sup>3</sup>; <sup>1</sup>*CapSenze HB, Lund, Sweden*; <sup>2</sup>*Genovis AB, Lund, Sweden*; <sup>3</sup>*Bruker Daltonik GmbH, Bremen, Germany*; <sup>4</sup>*Bruker Daltonics Ltd, Coventry, UK*; <sup>5</sup>*Bruker Daltonics Inc, Fremont, CA*; <sup>6</sup>*Bruker Daltonics Inc, Billerica, MA*
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- ThP 534 **Comprehensive Profiling of Protein Lysine Acetylation in Human Esophageal Carcinoma Cell SHEEC**; [Kai Zhang](#)<sup>1</sup>; Shanshan Tian<sup>1</sup>; Guijin Zhai<sup>1</sup>; Zhenchang Guo<sup>1</sup>; Zhongyi Cheng<sup>2</sup>; <sup>1</sup>*Tianjin Medical University, Tianjin, China*; <sup>2</sup>*PTM Biolabs, Inc, Hangzhou, China*
- ThP 535 **MS-based Quantitative Proteomics using SILAC Mouse Reveals the Rhythmicity of the Circadian PTMome in the Liver**; Loïc Dayon<sup>1</sup>; Daniel Mauvoisin<sup>2</sup>; [Antonio Núñez Galindo](#)<sup>1</sup>; Jingkui Wang<sup>3</sup>; Félix Naef<sup>3</sup>; Martin Kussmann<sup>1</sup>; Frédéric Gachon<sup>2</sup>; <sup>1</sup>*NIHS, Molecular Biomarkers, Lausanne, CH*; <sup>2</sup>*NIHS, Circadian Rhythm Group, Lausanne, CH*; <sup>3</sup>*Institute of Bioengineering, EPFL, Lausanne, CH*
- ThP 536 **Proteoform Dynamics in the CNS: 3D Spatial Mapping of Myelin Basic Protein by Top Down**; [Daniel Plymire](#); John Corbett; Steven Patrie; *University of Texas Southwestern Medical Center, Dallas, TX*
- ThP 537 **Identification of Liver Proteins Targeted by Reactive Metabolites using LC-MS/MS**; [Makan Golizeh](#); André Leblanc; Lekha Sleno; *UQAM, Montreal, Canada*
- ThP 538 **High Sensitivity LC-MS and LC-MS/MS Peptide Mapping Method for Characterization of Post-Translational Modifications in Therapeutic Antibodies**; Jason X. Tang; [Yuping Zhou](#); *Eli Lilly & Company, Indianapolis, IN*
- ThP 539 **Novel Activity Based Protein Profiling Probe Identifies Putative Dentrane in Microglia**; [Harris Bell-Temin](#)<sup>1, 2</sup>; Jennifer Guergues<sup>1</sup>; Annie Carpenter<sup>1</sup>; Christina Carlson<sup>1</sup>; Stanley M. Stevens Jr. <sup>1</sup>; <sup>1</sup>*University of South Florida, Tampa, FL*; <sup>2</sup>*University of Pittsburgh, Pittsburgh, PA*
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- ThP 596 **Enhanced Detection of Host-Cell Proteins in Biotherapeutic Preparations using Preparative Electrophoresis followed by LC – Ion Mobility – MS;** Chris Boles<sup>1</sup>; Brad J. Williams<sup>2</sup>; Bryan Spencer<sup>1</sup>; Danny Yun<sup>1</sup>; Sadaf Hoda<sup>1</sup>; <sup>1</sup>Sage Science, Inc., Beverly, MA; <sup>2</sup>Waters Corporation, Beverly, MA
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- ThP 603 **Differential Protein Precipitation of Therapeutic Monoclonal Antibody from Serum Albumin and Its Application for Antibody Bioanalysis by LC-MS/MS;** Hongyan Li; Linh Tran; Christopher James; *Amgen Inc, Thousand Oaks, CA*
- ThP 604 **Highly Sensitive LC-MS/MS Quantitation of Insulin Aspart in Human Plasma: Comparison of Intact and Enzymatic Digestion Approach;** Hui Hong; Chao Bian; Yi Tao; Xiaohang Shen; Wenzhong Liang; Xin Zhang; *WuXi AppTec (Shanghai) Co. Ltd., Shanghai, China*
- ThP 605 **Rapid Protein Digestion with Thermostable Chemically Modified Trypsin for Mass Spec-Based Protein Characterization and PK Studies;** Sergei Saveliev; Mark Bratz; Mike Rosenblatt; Nidhi Nath; Marjeta Urh; *Promega Corporation, Madison, WI*
- ThP 606 **Development of Simplified Quantitative Method for Tryptic Digested C-reactive Protein by using Online SPE Coupled to Triple Quadrupole Mass Spectrometer;** Tairo Ogura; Toshiya Matsubara; Ichiro Hirano; *Shimadzu Corporation, Kyoto, Japan*
- ThP 607 **Identification and Quantification of Host Cell Protein Impurities in High-Purity Monoclonal Antibodies Down to 1 ppm: An Inter-Laboratory Study;** Catalin Doneanu<sup>1</sup>; Malcolm Anderson<sup>3</sup>; Brad Williams<sup>2</sup>; Matthew Lauber<sup>1</sup>; Asish Chakraborty<sup>1</sup>; Markus Wanninger<sup>1</sup>; Patricia Young<sup>1</sup>; Weibin Chen<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Waters Corporation, Beverly, MA; <sup>3</sup>Waters Corporation, Manchester, UK
- ThP 608 **Development of a Targeted LC-MS/MS Assay for the Quantitation of Varicella Zoster Virus Vaccine Proteins;** Kristin Geddes; Colleen Price; Jianfang Hu; Eberhard Durr; Nwanyinma Nnodum; Jack Palmer; Jessica Sinacola; Kevin Bateman; Van Hoang; Daniel Spellman; *Merck and Co, Inc, West Point, PA*
- ThP 609 **A Novel Antibody-Free, Dual-Mechanism Enrichment Method for High-Throughput and Ultra-Sensitive Quantification of mAb;** Bo An; Ming Zhang; Yang Qu; Jun Qu; *SUNY at Buffalo, Buffalo, NY*
- ThP 610 **A Robust and Automated Generic Sample Extraction Method for Quantifying Antibody Therapeutics in Biological Matrices;** Suma Ramagiri<sup>1</sup>; Mike Rosenblatt<sup>2</sup>; Ian Moore<sup>1</sup>; Nidhi Nath<sup>2</sup>; Kevin Cook<sup>2</sup>; Gary Impey<sup>1</sup>; <sup>1</sup>SCIEX, Concord, Canada; <sup>2</sup>Promega Corporation, Madison, WI
- ThP 611 **Development of a Rapid and Robust LC-MS Assay for Host Cell Proteins;** Thomas Slaney<sup>1</sup>; Wei Wu<sup>1</sup>; Li Tao<sup>2</sup>; Lu Wang<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb, Bloomsbury, NJ; <sup>2</sup>Bristol-Myers Squibb, Hopewell, NJ
- ThP 612 **Validation of the Quantification of a Major Grass Pollen Allergen by Mass Spectrometry;** Emmanuel Nony; Christel Dayang; Matthieu Rouet; Sandrine Riandé; Maxime Le Mignon; Thierry Batard; Philippe Moingeon; *Stallergenes, Antony, France*
- ThP 613 **Detection and Quantification of Low-abundant GDF-11 in Nondepleted Biofluid Protein Complexity Using LCMS/MS and LCMS/MS Analysis;** Liming Peng<sup>1</sup>; Srinivasan Krishnan<sup>2</sup>; Xiaohong Chen<sup>1</sup>; Shalender Bhasin<sup>1</sup>; <sup>1</sup>Brigham and Women's Hospital, Boston, MA; <sup>2</sup>Ab Sciex, Foster City, CA
- ThP 614 **Evaluation of Affinity Capturing Techniques for the LC/MS Analysis of Biotherapeutics in Biological Matrices;** Dongliang Zhan<sup>1</sup>; Rand Jenkins<sup>1</sup>; William R. Mylott<sup>1</sup>; Patrick Bennett<sup>1</sup>; Urban Kiernan<sup>2</sup>; Kwasi Antwi<sup>2</sup>; Eric Niederkofler<sup>2</sup>; <sup>1</sup>PPD, Inc., Richmond, VA; <sup>2</sup>Thermo Fisher Scientific, Tempe, AZ
- ThP 615 **Targeted Mass Spectrometry for the Analysis of Biomarkers and Biopharmaceuticals;** Rainer Bischoff<sup>1</sup>; Kees Bronsema<sup>1</sup>; Daniel Wilffert<sup>1</sup>; Nico van de Merbel<sup>2</sup>; <sup>1</sup>University of Groningen, Groningen, Netherlands; <sup>2</sup>PRA Health Sciences, Assen, The Netherlands
- ThP 616 **Analysis of Bioreactor Proteins using High Throughput Data-Independent Acquisition;** Martha Stapels; Marcella Yu; Caroline DiCesare; Kevin Brower; Khanita Karaveg; Monica Lane; Xiaokui Kate Zhang; *Sanofi Biotherapeutics, Framingham, MA*
- ThP 617 **Enzyme Activity Assay of a PEGylated Arginase in Mouse Serum Using LC-MS/MS;** Oanh Dang<sup>1</sup>; Susan Alters<sup>2</sup>; Scott Rowlinson<sup>2</sup>; Everett Stone<sup>3</sup>; John Bruce<sup>1</sup>; Shannon Bryant<sup>1</sup>; Michael Buonarati<sup>1</sup>; Dale Schoener<sup>1</sup>; <sup>1</sup>Intertek Pharmaceutical Services, El Dorado Hills, Ca; <sup>2</sup>Aeglea Biotherapeutics, Austin, TX; <sup>3</sup>University of Texas at Austin, Austin, TX

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- ThP 618 **Single Analytical Tool for Establishing Biosimilarity: A Biosimilar Case Study;** Faraz Rashid; Annu Uppal; Dipankar Malakar; Manoj Pillai; *Sciex., 121, DHR holding Udyog Vihar Phase-4, HR*
- ThP 619 **Characterization of Innovator and Biosimilar Monoclonal Antibodies with Ion Mobility Q-TOF MS;** Koen Sandra<sup>1</sup>; Isabel Vandenheede<sup>1</sup>; David Wong<sup>2</sup>; Ken Imatani<sup>2</sup>; Pat Sandra<sup>1</sup>; <sup>1</sup>RIC, Kortrijk, Belgium; <sup>2</sup>Agilent Technologies, Inc., Santa Clara, CA
- ThP 620 **Application of Complementary HRMS Methodologies for a Thorough Biosimilar Comparability Assessment;** Kevoork Mekhssian; Jean-Nicholas Mess; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*
- ThP 621 **Can Human Therapeutics Antibody (Humira) be Analyzed by LC-MS/MS in Plasma without Affinity Enrichment?** Luca Genovesi; Jean-Nicholas Mess; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*
- ThP 622 **Disulfide Bond Mapping of Biosimilar Infliximab;** Annu Uppal<sup>1</sup>; Milla Neffling<sup>2</sup>; Steve Taylor<sup>2</sup>; Dipankar Malakar<sup>1</sup>; Faraz Rashid<sup>1</sup>; Manoj Pillai<sup>1</sup>; <sup>1</sup>SCIEX, 121, Udyog Vihar,

- Phase IV, Gurgaon, Haryana, India; <sup>2</sup>SCIEX, Phoenix House, Lakeside Drive, Warrington, Cheshire, UK
- ThP 623 **Intact Antibody Structural Characterization using H/D Exchange and Top-Down Electron Transfer Dissociation on an Orbitrap**; Jingxi Pan<sup>1</sup>; Suping Zhang<sup>1</sup>; Albert Chou<sup>1</sup>; Darryl Hardie<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada; <sup>2</sup>Dept. of Biochem. & Microbiol., Univ. of Victoria, Victoria, BC, Canada
- ThP 624 **Complete Primary Structure and Biosimilarity Assessment of Monoclonal Antibodies in a Single Analysis Using Transient Isotachopheresis Capillary Electrophoresis-Tandem Mass Spectrometry**; Rabah Gahoual<sup>1,3</sup>; Jean-Marc Busnel<sup>4</sup>; Alain Beck<sup>2</sup>; Yannis-Nicolas Francois<sup>1</sup>; Emmanuelle Leize-Wagner<sup>1</sup>; <sup>1</sup>LSMIS, UMR 7140, University of Strasbourg, Strasbourg, France; <sup>2</sup>Centre d'immunologie Pierre Fabre, Saint-Julien-en-Genevois, France; <sup>3</sup>University of Amsterdam, Amsterdam, Netherlands; <sup>4</sup>Beckman Coulter Inc, Marseille, France
- ThP 625 **Comprehensive Characterization of Etanercept including N-IO-Glycosylation and Disulfide Linkage using Novel Bioinformatics Software**; Anke Schnabel; Gerhard Koerting; Heiner Falkenberg; Yvonne Jasper; Andreas Wattenberg; *Protagen Protein Services GmbH, Dortmund, Germany*
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- ThP 627 **Determination and Analysis of Sulfur-Containing Compounds in Petroleum using Silver Cations and Ion Mobility- Mass Spectrometry (IM-MS) Instrumentation**; Hossein Maleki; Gregory Donohoe; Stephen Valentine; *West Virginia University, Morgantown, WV*
- ThP 628 **Ion Mobility Mass Spectrometry (IM-MS) Applications in Modern Agricultural Research**; Jeffrey Gilbert<sup>1</sup>; David Mccaskill<sup>1</sup>; Jesse Balcer<sup>1</sup>; Yelena A. Adelfinskaya<sup>1</sup>; Anthony P. Gies<sup>2</sup>; Suresh Babu Annangudi Palani<sup>1</sup>; Gerrit DeBoer<sup>1</sup>; Krishnamoorthy Kuppannan<sup>3</sup>; Mary Evenson<sup>1</sup>; Lisa Buchholz<sup>1</sup>; Bruce Bell<sup>3</sup>; <sup>1</sup>Dow AgroSciences, Indianapolis, IN; <sup>2</sup>Dow Chemical Company, Freeport, TX; <sup>3</sup>The Dow Chemical Company, Midland, MI
- ThP 629 **MS-Based Comparisons of Rituximab Drug Products: Influence of Instrument Resolution, Chromatography and Ion Mobility on Structural Characterization**; Ashley C. Gucinski; Carly Ferguson; Michaela Levy; Michael T. Boyne II; *U.S. FDA, Saint Louis, MO*
- ThP 630 **Profiling Complex E/L Polymer Mixtures Using Ion Mobility Mass Spectrometry, a Novel 4D Data Mining Algorithm and Differential Analysis Software**; David A. Weil<sup>1</sup>; Caroline S. Chu<sup>2</sup>; <sup>1</sup>Agilent Technologies, Schaumburg, IL; <sup>2</sup>Agilent Technologies, Inc, Santa Clara, CA
- ThP 631 **Microfluidic UPLC Ion Mobility: A New Approach to Authentication and Routine Screening of Ginsenoside Isomers in Functional Food Products**; Michael Mccullagh; John Chipperfield; Ramesh P Rao; David Douce; *Waters, Manchester, UK*
- ThP 632 **Structural Characterization of Isomeric Polymer Precursors by Electropray Ion Mobility-Mass Spectrometry and Computational Strategies**; Tiffany M. Onifer; Sarah M. Stow; Jay G. Forsythe; Jody C. May; John A. McLean; David M. Hercules; *Vanderbilt University, Nashville, TN*
- ThP 633 **Baby Elephants Can Surf: Using the Selectivity of Ion Mobility When Screening Multi-class Pesticides in Fruit and Vegetables**; Séverine Gosciny<sup>1</sup>; Michael McCullagh<sup>2</sup>; <sup>1</sup>Scientific Institute of Public Health, Brussels, Belgium; <sup>2</sup>Waters, Manchester, UK
- ThP 634 **Using the Routine Separation Dimension and Identification Criteria of Microfluidic UPLC Ion Mobility to Enhance Specificity in Screening Complex Samples**; Michael Mccullagh<sup>1</sup>; C.A.M Pereira<sup>2</sup>; J.H Yariwake<sup>2</sup>; David Douce<sup>1</sup>; <sup>1</sup>Waters (MS Technologies), Wilmslow, UK; <sup>2</sup>Universidade de Sao Paulo, Sao Paulo, Brazil
- ThP 635 **Ion Mobility Spectrometry - Mass Spectrometry Analysis of Home Made Explosive Components and Background Materials**; Nathan Hagan<sup>1</sup>; Ilana Goldberg<sup>1</sup>; Adam M Graichen<sup>2</sup>; Amanda St Jean<sup>1</sup>; Ching Wu<sup>2</sup>; Plamen A. Demirev<sup>1</sup>; <sup>1</sup>JHU Applied Physics Lab, Laurel, MD; <sup>2</sup>Excellims Corporation, Acton, MA
- ThP 636 **A Novel Strategy to Screen and Profile Steviol Glycosides of Natural Sweeteners in Food Using Microfluidic UPLC Ion Mobility**; Ramesh P Rao<sup>1</sup>; Michael McCullagh<sup>1</sup>; David Douce<sup>1</sup>; Séverine Gosciny<sup>2</sup>; <sup>1</sup>Waters Corporation, Manchester, UK; <sup>2</sup>Scientific Institute of Public Health, Brussels, Belgium
- ThP 637 **Analysis of Fruit Juice Samples with HPLC and CZE Coupled to IMS-qTOF-MS**; Susanne Stephan; Oliver J. Schmitz; *University of Duisburg-Essen, Essen, Germany*
- ThP 638 **The Effective Utilization of Shape Selective Information in the Characterisation of Complex Mixtures**; Imtiaaz Khan<sup>1</sup>; David Portwood<sup>2</sup>; Pablo Navarro<sup>2</sup>; Lou Mason<sup>2</sup>; Matthew Edgeworth<sup>1</sup>; James Scrivens<sup>1</sup>; <sup>1</sup>University of Warwick, Coventry, UK; <sup>2</sup>Syngenta, Bracknell, UK
- ThP 639 **Degradation Profile of Conventional and Full Synthetic Engine Oil During Normal Vehicle Operation using Ion Mobility Mass Spectrometry**; Christian Klein; Ed Darland; Ruwan Kurulugama; Bill Barry; George Stafford; *Agilent Technologies, Santa Clara, CA*
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- ThP 640 **Role of Alkali Metals and Buffer Gases for Fast Differentiation of Gonyautoxin Isomers by Ion Mobility - Mass Spectrometry**; Salomé Poyer<sup>1</sup>; Corinne Loutelier-Bourhis<sup>1</sup>; Florence Mondeguer<sup>2</sup>; Julien Enche<sup>3</sup>; Vincent Tognetti<sup>1</sup>; Laurent Joubert<sup>1</sup>; Anne Bossée<sup>3</sup>; Philipp Hess<sup>2</sup>; Carlos Afonso<sup>1</sup>; <sup>1</sup>University of rouen, Mont Saint Aignan, France; <sup>2</sup>Ifremer, Nantes, France; <sup>3</sup>DGA Maîtrise NRBC, Vert-le-petit, France
- ThP 641 **Evaluation of the Utility of Alternative Drift Gases in a Low Pressure Conventional Drift Tube Ion Mobility Mass Spectrometer**; Ruwan Kurulugama; George Stafford; Alex Mordehai; John Fjeldsted; *Agilent Technologies, Santa Clara, CA*
- ThP 642 **The Importance of Charge Isomers in Quantitation; Ion Mobility Mass Spectrometry of Fluoroquinolone Antibiotics**; Cris Laphorn<sup>1</sup>; Mike McCullagh<sup>2</sup>; Sara Stead<sup>2</sup>; Martin Palmer<sup>2</sup>; Kevin Giles<sup>2</sup>; Keith Richardson<sup>2</sup>; Jasper Boschmans<sup>3</sup>; Frank Sobott<sup>3</sup>; Frank Pullen<sup>1</sup>; Babur Chowdhry<sup>1</sup>; George Perkins<sup>4</sup>; <sup>1</sup>University of Greenwich, Chatham Maritime, UK; <sup>2</sup>Waters Corp, Manchester, UK; <sup>3</sup>University of Antwerp, Antwerp, Belgium; <sup>4</sup>149 Hickory Corner Road, Milford, NJ
- ThP 643 **Mining Secondary Metabolites by HPLC Chip Cube and Ion Mobility- Mass Spectrometry**; Nichole M. Lareau<sup>1</sup>; Sarah M. Stow<sup>1</sup>; Jody C. May<sup>1</sup>; Ed Darland<sup>2</sup>; Ruwan T. Kurulugama<sup>2</sup>; Emma E. Rennie<sup>2</sup>; John C. Fjeldsted<sup>2</sup>; John A. Mclean<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- ThP 644 **Distinguishing of Isobaric Compounds By Ion Mobility-Mass Spectrometry using Different Drift Gases and Mobility Peak Fitting**; Karel Lemr<sup>1</sup>; Martina Hermannová<sup>2</sup>; Lucie Borovcová<sup>1</sup>; Kristína Slováková<sup>1</sup>; Sandra Benická<sup>1</sup>; Vladimír Havlíček<sup>3</sup>; <sup>1</sup>RCPTM, Palacky University, Olomouc, Czech Republic; <sup>2</sup>Contipro Pharma, a.s., Dolní Dobruč, Czech Republic; <sup>3</sup>Institute of Microbiology, v.v.i., Prague, Czech Republic





- ThP 645 **Rapid Identification of Pathogenic *Naegleria* in Drinking Water Systems using Ion Mobility-Mass Spectrometry;** Zhihao Yu<sup>1</sup>; Xing Zhang<sup>1</sup>; Haylea Miller<sup>2</sup>; Geoffrey Puzon<sup>2</sup>; Brian Clowers<sup>1</sup>; <sup>1</sup>Washington State University, Pullman, WA; <sup>2</sup>CSIRO Land and Water, Perth, Australia
- ThP 646 **Demonstration of Collisional Cross Section Value Conservation across LC and GC Analyses;** Lauren Mullin<sup>1,2</sup>; Gareth Cleland<sup>2</sup>; Mike McCullagh<sup>3</sup>; Ingrid Ericson Jogsten<sup>1</sup>; <sup>1</sup>MTM Research Centre Örebro University, Örebro, Sweden; <sup>2</sup>Waters Corporation, Milford, MA; <sup>3</sup>Waters Corporation, Wilmslow, UK
- ThP 647 **Ion Mobility Data in Metabolite Identification: A Mass-MetaSite Approach;** Ismael Zamora<sup>1</sup>; Kevin Bateman<sup>3</sup>; Fabien Fontaine<sup>4</sup>; Russell Mortishire<sup>2</sup>; Ian McIntosh<sup>3</sup>; <sup>1</sup>Lead Molecular Design, S.L., Sant Cugat Del Valles, SPAIN; <sup>2</sup>Waters Corp, Milford, MS; <sup>3</sup>Merck, West Point, PN; <sup>4</sup>Molecular Discovery, London, UK
- ThP 648 **Multidimensional Analytical Approaches: Combining Ion Mobility and Spectrophotometric Detection with Current MS-based Metabolomics and Lipidomics Workflows;** Giuseppe Paglia<sup>1</sup>; Tommaso Pacini<sup>2</sup>; Steinn Gudmundsson<sup>2</sup>; A Eugenio Chiaravalle<sup>1</sup>; Sigurdur Brynjolfsson<sup>2</sup>; Bernard O Palsson<sup>2</sup>; Giuseppe Astarita<sup>3</sup>; <sup>1</sup>IZS Puglia e Basilicata, Foggia, Italy; <sup>2</sup>Center For Systems Biology, Reykjavik, Iceland; <sup>3</sup>Waters Corporation, Milford, MA
- ThP 649 **The Analysis of Bile Acids: Enhancement of Specificity using an Ion Mobility-TOFMS Based Approach;** Jonathan P. Williams<sup>1</sup>; Jonas Abdel-Khalik<sup>2</sup>; Yuqin Wang<sup>2</sup>; Sarah M. Stow<sup>3</sup>; Mark Towers<sup>1</sup>; Giuseppe Astarita<sup>1</sup>; James Langridge<sup>1</sup>; William J. Griffiths<sup>2</sup>; <sup>1</sup>Waters, Manchester, UK; <sup>2</sup>College of Medicine, Swansea, UK; <sup>3</sup>Vanderbilt University, Nashville, TN, USA, Nashville, TN
- ThP 650 **Separation and Characterization of Native and Modified Oligonucleotides by Differential Mobility Separation Mass Spectrometry (DMS-MS);** Zhidan Chen<sup>1</sup>; Stephen Coy<sup>1</sup>; Albert Fornace<sup>2</sup>; Paul Vouros<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Georgetown University, Washington, DC
- ThP 651 **Structural Mass Spectrometry in Origins-of-Life Research: Abiotic Peptide Formation and Evolution;** Facundo Fernandez<sup>1</sup>; Jay Forsythe<sup>1</sup>; Sheng-Sheng Yu<sup>1</sup>; Ramanarayanan Krishnamurthy<sup>2</sup>; Martha Grover<sup>1</sup>; Nicholas Hud<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA; <sup>2</sup>The Scripps Research Institute, La Jolla, CA
- ThP 652 **Method Development in Selective Separation of Isomeric Small Molecules in Complex Matrices on IMS/Q-TOF Platform;** Christopher Beekman; Christopher Chouinard; Richard A. Yost; *Department of Chemistry, University of Florida, Gainesville, FL*
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- ThP 653 **A Hybrid MSI Method Combining MALDI and NIMS for Small Molecule Discovery and Identification in Crustacean Brain Tissue;** Chuanzi Ouyang<sup>1</sup>; Qinjingwen Cao<sup>1</sup>; Lingjun Li<sup>1,2</sup>; <sup>1</sup>Department of Chemistry, UW-Madison, Madison, WI; <sup>2</sup>School of Pharmacy, UW-Madison, Madison, WI
- ThP 654 **AFM-sampling-L<sup>2</sup>MS on Painting Cross-Sections;** Mark Little<sup>1</sup>; Craig Prater<sup>1</sup>; Eoghan Dillon<sup>1</sup>; Shawn Owens<sup>2</sup>; Jacob Berenbeim<sup>2</sup>; Catherine Patterson<sup>3</sup>; Mattanjah de Vries<sup>2</sup>; <sup>1</sup>Anasys Instruments, Santa Barbara, CA; <sup>2</sup>University of California Santa Barbara, Santa Barbara, CA; <sup>3</sup>Getty Conservation Institute, Los Angeles, CA
- ThP 655 **Improvements in Biomolecular Analysis with Secondary Ion Mass Spectrometry of Bacteria, Brain and Breast Cancer Samples;** Tina Angerer<sup>1</sup>; Masoumeh Dowlatshahi Pour<sup>2</sup>; Patrick Wehrli<sup>1</sup>; Per Malmberg<sup>2</sup>; John Fletcher<sup>1,2</sup>; <sup>1</sup>University of Gothenburg, Gothenburg, Sweden; <sup>2</sup>Chalmers University of Technology, Sweden, Gothenburg, Sweden
- ThP 656 **Imaging of Kidney Allograft Biopsies Combining TOF-SIMS and MALDI-TOF Spectrometers: From Methodological Study to the Research of Rejection Biomarkers;** Manale Noun<sup>1</sup>; Jean Pierre Le Caer<sup>1</sup>; David Touboul<sup>1</sup>; Dany Anglicheau<sup>2,3</sup>; Marion Rabant<sup>2,4</sup>; Pierre Marquet<sup>5</sup>; Alain Brunelle<sup>1</sup>; <sup>1</sup>Institut de Chimie des Substances Naturelles, CNRS, Gif Sur Yvette, France; <sup>2</sup>INSERM U1151, Paris, France; <sup>3</sup>Néphrologie et transplantation adulte, Necker hosp, Paris, France; <sup>4</sup>Lab. d'anatomie pathologique, Necker hosp, Paris, France; <sup>5</sup>UMR 850 Inserm. Université de Limoges, Limoge, France
- ThP 657 **Visualizing and Identifying Peptides Associated with Regenerating Tissue via Mass Spectrometry;** Ta-Hsuan Ong; James Collins; Rachel Roberts-Galbraith; Elena Romanova; Phillip Newmark; Jonathan Sweedler; *University of Illinois at Urbana-Champaign, Urbana, IL*
- ThP 658 **Practical Bioimaging using Massive Cluster Impact SIMS in a Time-of-Flight Ion-Microscope;** Jitao Zhang; Klaus Franzreb; Sergei Aksyonov; Peter Williams; *Tempe, AZ*
- ThP 659 **Imaging Mass Spectrometry Analysis and Comparison of Metal, Lipid, and Protein Distributions in Biological Tissues;** Christopher Shiea<sup>1</sup>; Hung Su<sup>2</sup>; Shiang-Jiun Lin<sup>2</sup>; Yeou-Lih Huang<sup>1</sup>; Jentaie Shiea<sup>2</sup>; <sup>1</sup>Kaohsiung Medical University, Kaohsiung, Taiwan; <sup>2</sup>National Sun Yat-Sen University, Kaohsiung, Taiwan
- ThP 660 **Integration of MS Imaging and Proteomic Data for Biological Discovery in a 3D Microtissue Model of Colon Cancer;** Peggy M. Angel; Linda Prengaman; Christina Lee; Erin Seeley; *Protea Biosciences, Morgantown, WV*
- ThP 661 **Improved Submicron Spatial Resolution of Thermal Desorption Mass Spectrometry via Short Tailored Pulse Heating with Thermal AFM Probes;** Suhas Somnath<sup>1</sup>; Stephen Jesse<sup>1</sup>; Gary J. Van Berkel<sup>2</sup>; Sergei V. Kalinin<sup>1</sup>; Olga Ovchinnikova<sup>2</sup>; <sup>1</sup>CNMS, Oak Ridge National laboratory, Oak Ridge, TN; <sup>2</sup>OBMS, Oak Ridge National laboratory, Oak Ridge, TN
- ThP 662 **Verifying Continuity of Membranous Organelles and Measurements of Exchange Rate Between the Nucleus and Cytoplasm using FLIP-Like MALDI-Based Imaging;** A. Jablolkow<sup>1</sup>; O. Gradow<sup>2</sup>; <sup>1</sup>National Research Medical University, Moscow, RF; <sup>2</sup>Institute of Energy Problems of Chemical Physics, Moscow, RF
- ThP 663 **Drugs of Abuse in Hair Sections Examined at High Resolution by TOF-SIMS Imaging;** Gregory Fisher<sup>1</sup>; Bryn Flinders<sup>2</sup>; Eva Cuypers<sup>3</sup>; Ron Heeren<sup>2</sup>; <sup>1</sup>Physical Electronics, Chanhassen, MN; <sup>2</sup>M4I, Maastricht University, Maastricht, the Netherlands; <sup>3</sup>KU Leuven Toxicology and Pharmacology, Leuven, Belgium
- ThP 664 **Multimodal Imaging of Subpopulations in Cultured Cell Samples after Cell Transfection;** Sanna Sämfors<sup>1</sup>; Andreas Svanström<sup>2</sup>; John Fletcher<sup>1</sup>; Julie Grantham<sup>2</sup>; Andrew Ewing<sup>1</sup>; <sup>1</sup>Chalmers University of Technology, Gothenburg, Sweden; <sup>2</sup>University of Gothenburg, Gothenburg, Sweden
- ThP 665 **Single-Cell MALDI-TOF MS Profiling of Mammalian Islet of Langerhans;** Troy Comi; Erik Jansson; Ta-Hsuan Ong; Stanislav Rubakhin; Jonathan Sweedler; *University of Illinois at Urbana-Champaign, Urbana, IL*
- ThP 666 **Quantitative Imaging of Peptides on Mouse Brain Tissues by MALDI;** Kyung Man Park<sup>1</sup>; Jeong Hee Moon<sup>2</sup>; Seong Hoon Lee<sup>1</sup>; Myung Soo Kim<sup>1</sup>; <sup>1</sup>Seoul National University, Seoul, Korea; <sup>2</sup>Medical Proteomics Research Center, KRIBB, Daejeon, Korea
- ThP 667 **Phospholipid localization by Cold Cell LA-ICP-MS Imaging of Arabidopsis Thaliana Seeds and Extraction for Analysis by NSI-MS;** Emma Gorishek; Phillip Mach; Jason Hamilton; Guido Verbeck; *University of North Texas, Denton, TX*

- ThP 668 **Single Cell Analysis using High Spatial Resolution and High Sensitivity Imaging Mass Spectrometry;** Bo Yang<sup>1</sup>; Audra Judd<sup>1</sup>; David M. Anderson<sup>1,3</sup>; Jeffrey Spraggins<sup>1</sup>; Richard M. Caprioli<sup>1,2</sup>; Jeremy L. Norris<sup>1</sup>; <sup>1</sup>Vanderbilt University MSRC, Nashville, TN; <sup>2</sup>Department of Biochemistry, Nashville, TN; <sup>3</sup>Vanderbilt University School of Medicine, Nashville, TN
- ThP 669 **Increasing Spatial Resolution of Lipid Biomarker Analysis by LDI FT-ICRMS;** Lars Wörmer<sup>2</sup>; Susanne Alfkens<sup>2</sup>; Marcus Elvert<sup>2</sup>; Jens Fuchser<sup>1</sup>; Julius S. Lipp<sup>2</sup>; Matthias Zabel<sup>2</sup>; Kai-Uwe Hinrichs<sup>2</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup>MARUM, Bremen, Germany
- ThP 670 **Single Cell Analysis of Rat Brain Glia using MALDI-MSI and CE-MS;** Stanislav Rubakhin; Monika Makurath; Jonathan Sweedler; *University of Illinois, Urbana, IL*
- ThP 671 **Sub-micrometer Resolution Near-Field Laser Ablation Sample Transfer Mass Spectrometry of Cells and Tissue;** Suman Ghorai; Chinthaka A. Seneviratne; Kermit K. Murray; *Louisiana State University, Baton Rouge, LA*
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June 5 - 9, 2016

San Antonio, Texas

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