Welcome to the 65th ASMS Conference on Mass Spectrometry and Allied Topics. Conference program activities and exhibit booths are in the Indiana Convention Center. Corporate Member hospitality suites are located in the JW Marriott Hotel.

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ASMS gratefully acknowledges the support of these companies.

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Welcome Reception

SHIMADZU

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Closing Event

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Advanced Energy

TABLE OF CONTENTS

Titles in the following sections are provided by authors. The complete abstracts are available online at www.asms.org

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

Attention Undergraduate Students and First Time (at ASMS) Graduate Students

4:00 - 4:45 pm, Sunday, Room 107-110, level 1
Plan Your Strategy: What to See and Do at ASMS

TUTORIALS

Sunday Tutorial Session I, 5:00 - 6:30 pm

Hall D, level 1

5:00 - 5:45 pm
MALDI: Past and Future

Kermit K. Murray
Louisiana State University

5:45 - 6:30 pm
Cancer Immunotherapy and Mass Spectrometry

Donald F. Hunt
University of Virginia

Sunday Tutorial Session II, 5:00 - 6:30 pm

Wabash, level 1

5:00 - 5:45 pm
Ion Mobility Spectrometry: Analyzing Molecules as They Tumble through Life

Erin S. Baker
Pacific Northwest National Laboratory

5:45 - 6:30 pm
CE/MS - Ready for Prime Time?

Norman J. Dovichi
University of Notre Dame

PLENARY SESSIONS

Sunday Plenary Session, 6:45 - 7:45 pm

Hall D, level 1

Welcome

Richard A. Yost
University of Florida
ASMS Vice President for Programs

Towards a Good Start in Life: Neonatal Screening and Beyond

David S. Millington
Duke University Medical Center

Sunday Welcome Reception, 7:45 - 9:00 pm

Poster/Exhibit Hall. Conference name badge is required.

Monday Award Lecture, 4:45 - 5:30 pm

Hall D, level 1

Award for a Distinguished Contribution in Mass Spectrometry

Catherine E. Costello
Boston University

Tuesday Award Lecture, 4:45 - 5:30 pm

Hall D, level 1

Biemann Medal

Ryan Julian
University of California, Riverside

Thursday Plenary Session, 4:45 - 5:30 pm

Hall D, level 1

Saving the Great Coral Reefs

Kristen Marhaver
Research Station Carmabi

Thursday Closing Event at the Indiana State Museum, 6:30-9:00 pm, $30/person

Tickets must be purchased in advance by Monday 12 noon.

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 D
Session B (MOB, TOB, WOB, ThOB)..... 500 Ballroom
Level 2
Session C (MOC, TOC, WOC, ThOC).....Sagamore 1-3
Session D (MOD, TOD, WOD, ThOD).....Sagamore 4
Session E (MOE, TOE, WOE, ThOE).....Sagamore 5-7
Level 1
Session F (MOF, TOF, WOF, ThOF) ..... Wabash
Session G (MOG, TOG, WOG, ThOG).....Room 101-106
Session H (MOH, TOH, WOH, ThOH).....Room 107-110

Oral Presentations are projected from ASMS computers running Microsoft Office. 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 ready room is 117, level 1. 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 Welcome Reception....7:45 pm - 9:00 pm
Monday - Wednesday .....7:30 am - 8:00 pm
Thursday .....7:30 am - 2:30 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 2 and level 3.

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.

Free Wifi Access and Internet Stations are available throughout the convention center.

Conference Proceedings will be published online. Submission to the proceedings does not constitute publication and does not jeopardize the rights of authors to publish contents of their submissions. **Speaker slides will be printed to PDF and used as proceedings submission for speakers who fail to submit on their own.**

Webcasting includes tutorial lectures, plenary lectures, and oral sessions. Webcasts will be available to conference attendees for three months after the conference. ASMS does not retain rights to material included in webcasts.

Corporate Hospitality Suites may be open 8:00 – 10:30 pm, Monday through Wednesday. Suites are located in the **JW Marriott Hotel.**

Career Center is located in the Poster/Exhibit Hall. 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 welcome reception. The badge does not gain entrance to oral sessions or the Poster/Exhibit Hall.

Single Use/Family Restrooms are available on each level.

Mother's Room is Room 208, level 2 (for mothers-only).

Two Important Opportunities in the Poster/Exhibit Hall

1. **INFORMATICS HUB**
   Meet up with experts to discuss your infomatics questions.
2. **FUNDING AGENCY "OFFICE HOURS"**
   Consult with program officers and representatives from the major U.S. funding agencies.

Visit the *JASMS* booth number 111

1. Meet the Editor
2. Learn about submitting your ASMS presentation for publication

Conference Regulations

Please review these policies which are intended to assure the comfort and privacy of all conference participants.

Name badge is required for all conference sessions, including the Poster/Exhibit Hall and Career Center, and off site events such as the hospitality suites and closing event (ticket required).

No smoking is permitted in the convention center.

All devices must be silenced and screens darkened in oral sessions.

No photography or recording is allowed in oral sessions or in the poster/exhibit Hall.

Parents. Planned conference sessions and hospitality suites may not be appropriate for children. Please respect the interests of your colleagues by allowing them to attend activities without disruption and without concern for the safety of children. Strollers, child backpack carriers or similar devices for child transport are prohibited in the Poster/Exhibit Hall and hospitality suites.

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 express written authority of the author.

The placement of advertising in the meeting area is prohibited. There are poster boards and tables in the Poster/Exhibit Hall for approved announcements.

Hardware, accessories or any items for sale may be displayed only in corporate exhibit booths and hospitality suites.

Designated publisher tables in the conference registration area are for the display of books and journals and must be reserved in advance.

There are tables in the registration area for authors who wish to display their books. Authors may use a table to promote their books, sign copies, and speak with members. Table space must be reserved at conference registration.

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 hospitality suites may be used during the daytime hours of 8:00 am - 8:00 pm for one-on-one and small group meetings (no more than 25 persons per organization) by appointment only (no walk-ins). No music, programs, seminars, or refreshments may be included in these private, business meetings.

Corporate or institutional logos on slides or posters may appear only one time in the presentation.

Hotel	Telephone
JW Marriott	(317) 860-5800
Marriott Downtown	(317) 822-3500
Westin	(317) 262-8100
Hyatt Regency	(317) 632-1234
Omni Severin	(317) 634-6664
Crowne Plaza	(317) 631-2221

Hotel	Telephone
Hampton Inn & Suites	(317) 856-1000
Courtyard by Marriott	(317) 822-9029
Fairfield Inn & Suites (downtown)	(317) 636-7678
Springhill Inn (downtown)	(317) 972-7293
Hilton Garden Inn (downtown)	(317) 955-9700
Homewood Suites (downtown)	(317) 636-7992

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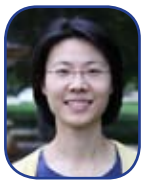

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to these members who were elected to the ASMS Board

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Interest Group Coordinators

Analytical Laboratory Managers	Emily Chen Aliss Chien
Bioinformatics for MS	Meena Choi Samuel Payne
Biotherapeutics	Charles Cheng Ashley Gucinski Ruth
Clinical Chemistry	Tim Garrett
Data Independent Acquisition	Ben Collins Ludovic Gillet
Drug Metabolism & Pharmacokinetics	Mark Cancilla Philip Tiller
Energy, Petroleum & Biofuels	Mark Barrow David Stranz
Environmental Applications	Marc Engel Achille Cappiello
Exposomics	H. M. Skip Kingston Anthony Macherone
Flavor, Fragrance and Foodstuff	Sara Kern David Schroeder
Forensics & Homeland Security	Kenyon Evans-Nguyen Adam Hall
FTMS	Melinda McFarland David Kilgour
Fundamentals	Victor Ryzhov Michael Van Stipdonk
H/D Exchange, Covalent Labeling & Cross Linking	Lan Huang David Weis
Imaging MS	Reid Groseclose Raf Van de Plas
Ion Mobility MS	Valerie Gabelica Stephen Valentine
Ion Trap MS	Zheng Ouyang Wei Xu
Lipids & Lipodomics	Eva Duchoslav Todd Mitchell
LC/MS Related Topics	Eric Soderblom Will Thompson
Metabolomics	John Bowden Tim Garrett
Metal Ion Coordination Chemistry	Eric Dodds Cheng Lin
Oligonucleaotides & Nucleic Acids	Patrick Limbach Laixin Wang
Pharmaceuticals	Matthew Schenauer John Valliere-Douglass
Photoionization MS	Eleanor Riches Ralf Zimmerman
Polymeric Materials	Christina Mastromatteo Stephen Rumbelow
Regulated Bioanalysis	Fabio Garofolo Jian Wang

Interest Group Coordinators (*continued*)

Undergraduate Research in MS	Megan Gessel James Pesavento
Young Mass Spectrometrists	Violet Lee Doug Phanstiel

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Nominating	Gary Glish, Chair Kristina Håkansson Lars Konermann Roy Martin Ljiljana Pasa-Tolic
Publications	Facundo Fernandez, Chair Lorna De Leoz Valerie Gabelica Jody C. May Will Thompson Joseph Loo (*ex officio*)
Sanibel Conference	Melinda McFarland Fanyu Meng Victor Ryzhov Ying Ge (ASMS Board Rep.)

AWARD FOR A DISTINGUISHED CONTRIBUTION IN MASS SPECTROMETRY

2017 Recipient: Catherine E. Costello

Award Lecture: 4:45 pm, Monday, Hall D, Level 1

Dr. Catherine E. Costello is the recipient of the 2017 Award for a Distinguished Contribution in Mass Spectrometry for her pioneering contributions to the development of tandem mass spectrometry of glycans and glycoconjugates.

Glycans differ from proteins in that their biosynthesis derives from a series of enzymatic reactions in the endoplasmic reticulum and Golgi apparatus and not from a template-driven process. Glycans, depending on class, may be branched, meaning that their structural determination requires determination of linkage positions and stereochemistry. The function of a glycan depends on the target to which it binds. A difference in a single monosaccharide linkage in a glycan alters the partners to which a glycan or glycoconjugate binds. For glycoproteins, the large number of proteoforms reflect glycan heterogeneity at each glycosylation site. Thus, the population of glycoprotein proteoforms present at any given place or time differ in their capacities to bind to partners that contain carbohydrate binding domains. The complexity of glycan and glycoconjugate structures presents a severe analytical challenge to the field of glycomics.

Prof. Costello's research has revolutionized glycomics by enabling comprehensive structural characterization of free glycans and glycoconjugates in a sensitive and high throughput fashion. In the 1980s she was among the first to recognize the potential of combining emerging soft ionization techniques with tandem mass spectrometry for characterization of glycans. Today, her 1988 publication defining the dissociation nomenclature for glycans remains highly cited. Prof. Costello delineated the strategy of producing the greatest degree of structural detail on glycans in a single tandem mass spectrometry step. She recognized that while collisional dissociation provides useful information, its utility is limited by low abundances of key cross-ring cleavage product ions. She developed activated electron dissociation methods for glycans and glycoconjugates that are inherently more effective for producing cross-ring cleavages. This has included studies of dissociation mechanisms and influences of metal cationization. Prof. Costello and her co-workers also pioneered Fourier Transform mass spectrometry of glycans and glycoconjugates with the application of electron based activation/dissociation methods and demonstrated these methods on a time scale compatible with on-line LC-tandem MS. Prof. Costello was the first to demonstrate top-down tandem MS analysis of intact glycoproteins. This is significant because most cell surface and secreted proteins are glycosylated and progress in biomedicine depends on the ability to characterize glycosylated proteoforms.

Prof. Costello's research activities define the present state of the art in glycan and glycoconjugate tandem mass spectrometry. These achievements address the needs in biomedicine for high throughput sequencing of glycans and glycoconjugates and for top-down analysis of intact glycoproteins.

Dr. Catherine E. Costello is a William Fairfield Warren Distinguished Professor, Department of Biochemistry, Cell Biology & Genomics, Department of Physiology & Biophysics, and Department of Chemistry, Boston University, Boston, MA.

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

Award Presentation: ASMS Meeting, 4:45 pm Wednesday, Sagamore 5-7, level 2

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 certificates.

The 2017 Award recognizes Thomas Rizzo, École Polytechnique Fédérale de Lausanne and co-authors for their paper **Infrared Spectroscopy of Mobility-Selected H+-Gly-Pro-Gly-Gly (GPGG)**; Antoine Masson[1], Michael Z. Kamrath[1], Marta A. S. Perez[1], Matthew S. Glover[2], U. Röthlisberger[1], David E. Clemmer[2], Thomas R. Rizzo[1]; [1]École Polytechnique Fédérale de Lausanne, [2]Indiana University; *JASMS* Vol. 26, Sept 2015, pp. 1444-1454

Antoine Masson

Michael Kamrath

Marta Perez

Matthew Glover

Ursula Rothlisberger

David Clemmer

Thomas Rizzo

BIEMANN MEDAL
2017 Recipient: Ryan Julian
Award Lecture: 4:45 pm Tuesday, Hall D, level 1

Dr. Ryan Julian is awarded the 2017 Biemann Medal for contributions related to his work developing and exploiting photo-initiated gas phase radical ion chemistry to probe peptide and protein structure. Several applications that rely on this chemistry have been developed by Ryan's lab including methods for (1) examining 3D protein structure in the gas phase, (2) site specific identification of Ser or Thr phosphorylation, (3) identification of Cys residues and disulfide pairs, (4) identification of peptide epimers, (5) oligosaccharide characterization, and (5) monitoring energy transfer with UV action spectra.

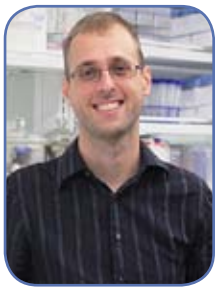
Prof. Julian has developed bond selective chemistry for initiating controllable radical directed dissociation (RDD). This is accomplished by photoexcitation with ultraviolet photons, leading to homolytic dissociation of specific bonds and the generation of a radical species. For example, photodissociation of carbon-iodine bonds with 266 nm photons occurs with high yield due to excitation of a dissociative excited state. If the carbon is covalently attached to a protein, then a radical is generated at that atom, and iodine radical is lost. The Julian lab has demonstrated that this chemistry can be used to create radicals in various types of biomolecules via dissociation of carbon-iodine, carbon-sulfur, and sulfur-sulfur bonds associated with numerous chromophores. Importantly, any of these bonds can be photodissociated regardless of molecular size, charge state, charge polarity, or sequence. The specificity inherent with this method allows for precise placement of an active radical in a controllable location, which can subsequently initiate fragmentation of the molecule via radical directed dissociation.

Dr. Julian is a professor in the Department of Chemistry at the University of California, Riverside.

2017 RESEARCH AWARDS
Award Presentation: 4:45 pm Tuesday, Hall D, level 1

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

Sponsored by
Thermo Fisher Scientific



Peter Nemes
The George Washington University

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Waters Corporation

Abraham Badu-Tawiah
The Ohio State University

2017 POSTDOCTORAL CAREER DEVELOPMENT AWARDS

Award Presentation: ASMS Meeting, 4:45 pm Wednesday, Sagamore 5-7, level 2

Five 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.

Bushra Amin
University of Pittsburgh

Andrea Carra
University of Minnesota

Romel P. Dator
University of Minnesota

Charles M. Nichols
Vanderbilt University

Wen-Jing Zhang
Wayne State University

2017 STUDENT AWARDS

Award Presentation: ASMS Meeting, 4:45 pm Wednesday, Sagamore 5-7, level 2

ASMS supports up to ten 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. The deadline for submission is January 15.

Graduate Student Awards

Melissa Budelier, Washington University

Bifan Chen, University of Wisconsin-Madison

Bingming Chen, University of Wisconsin-Madison

James Dodds, Vanderbilt University

Paul Hutchins, University of Wisconsin-Madison

Rosemary Onjiko, George Washington University

Elizabeth Peuchen, University of Notre Dame

Lindsay Pino, University of Washington

Matthew Waas, Medical College of Wisconsin

Emily Werth, Univeristy of North Carolina

Undergraduate Student Awards

Giovanni Calderisi, University of Innsbruck

Jack Clemmensen, Saint Mary's College of California

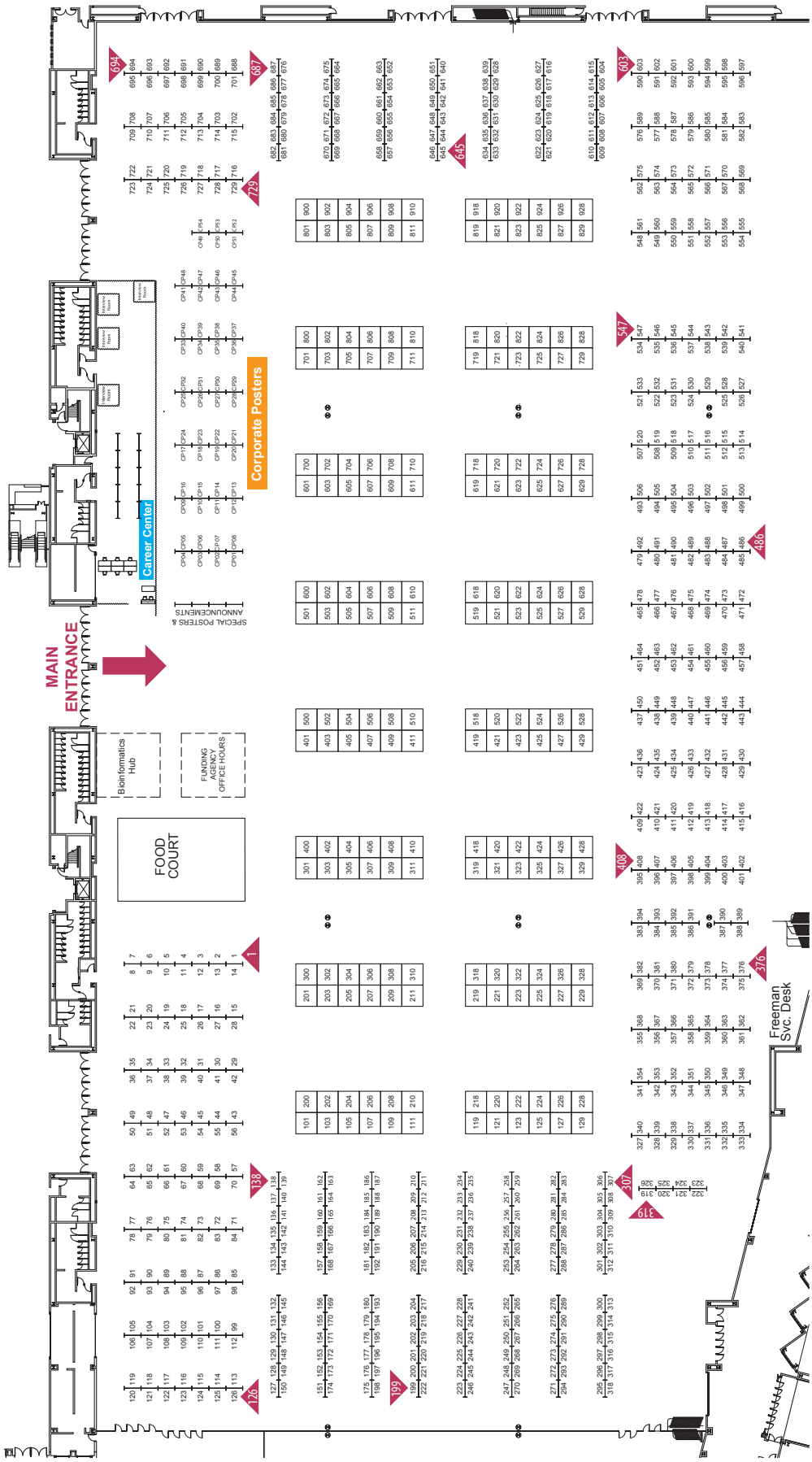
Jason Cochran, University of Florida

Mirna Giron, Kean University

Christopher Gongar, University of Florida

Shilpa Kolachina, University of Illinois at Chicago

John Lin, University of Texas at Austin


MAIN ENTRANCE
Bioinformatics Hub
FUNDING AGENCY OFFICE HOURS
FOOD COURT
Career Center
Corporate Posters
SPECIAL POSTERS & ANNOUNCEMENTS
Freeman Svc. Desk

Level 1

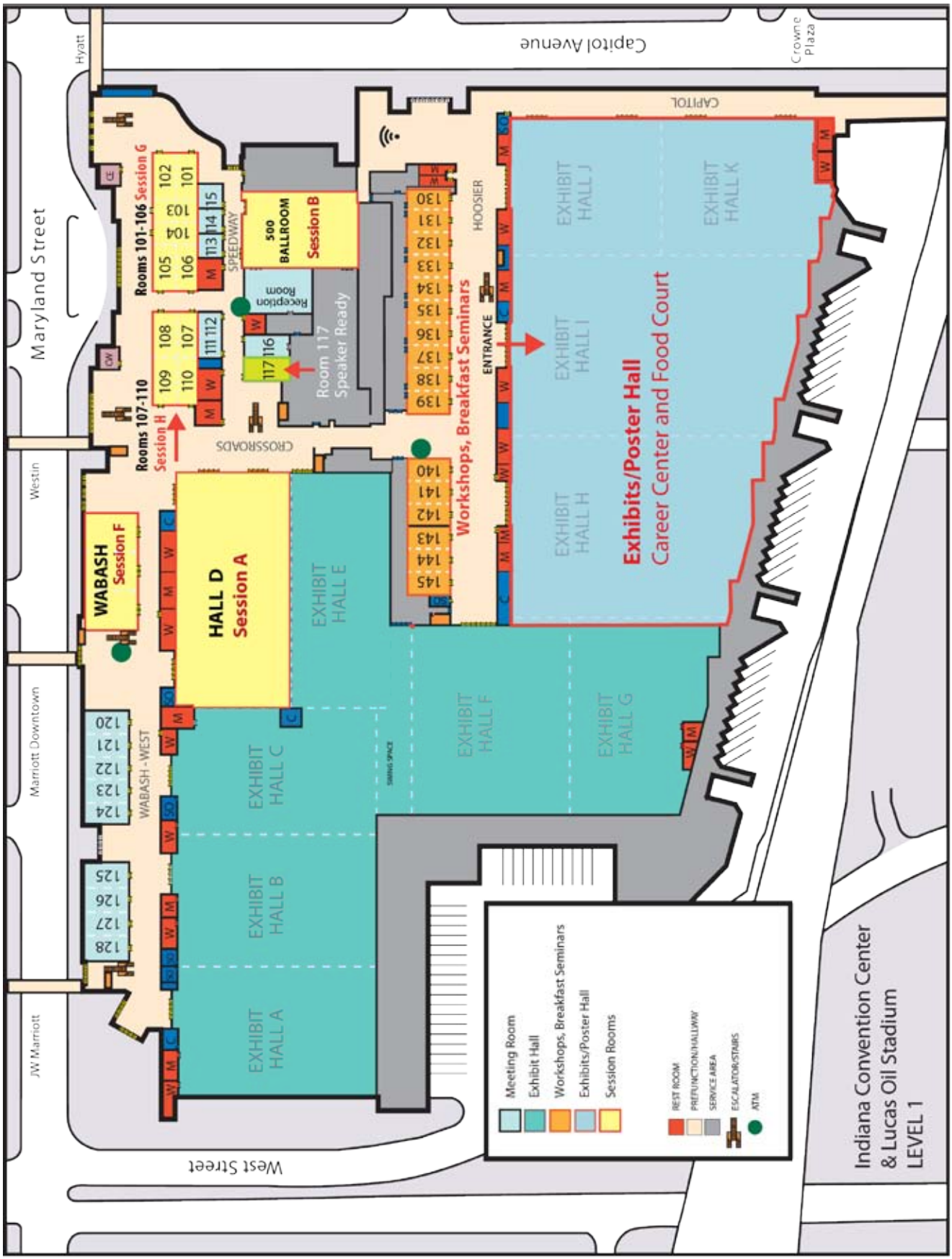

Capitol Avenue
Hyatt
Crowne Plaza
Maryland Street
Westin
Marriott Downtown
JW Marriott
West Street
CAPITOL
HOOSIER
SPEEDWAY
CROSSROADS
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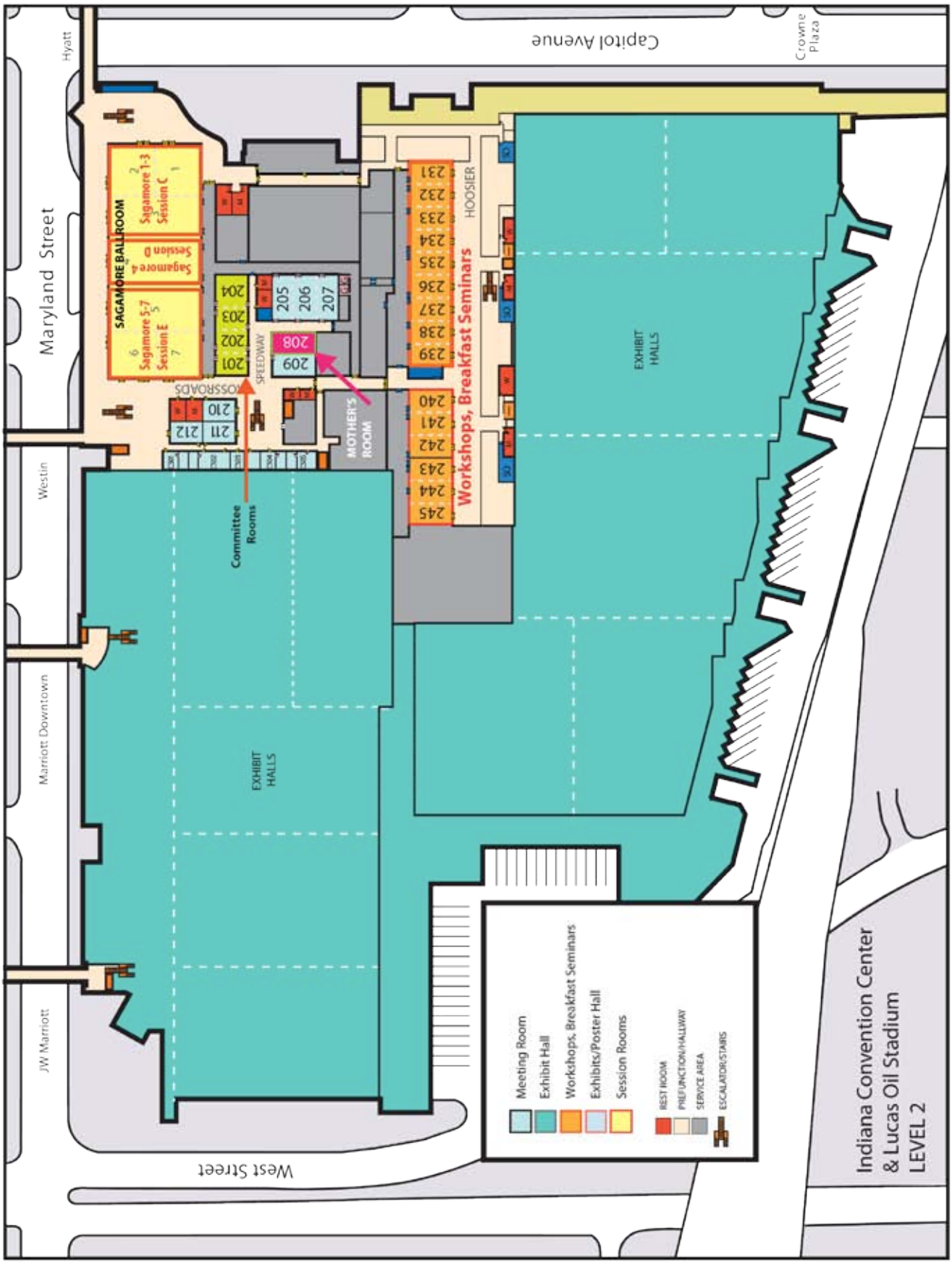
Exhibit Hall
Workshops, Breakfast Seminars
Exhibits/Poster Hall
Session Rooms
REST ROOM
PREFUNCTION/HALLWAY
SERVICE AREA
ESCALATOR/STAIRS
ATM

Level 2


Capitol Avenue
Hyatt
Crowne Plaza
Maryland Street
Westin
Marriott Downtown
JW Marriott
West Street
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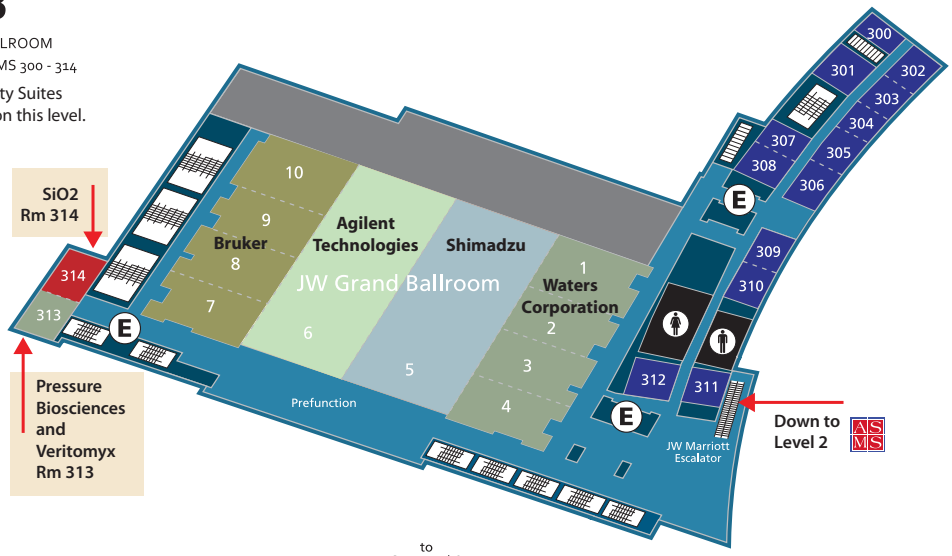
Workshops, Breakfast Seminars
Exhibits/Poster Hall
Session Rooms
REST ROOM
PRE/FUNCTION/HALLWAY
SERVICE AREA
ESCALATOR/STAIRS
Indiana Convention Center & Lucas Oil Stadium
LEVEL 2

LEVEL 3

JW GRAND BALLROOM
MEETING ROOMS 300 - 314

Hospitality Suites located on this level.

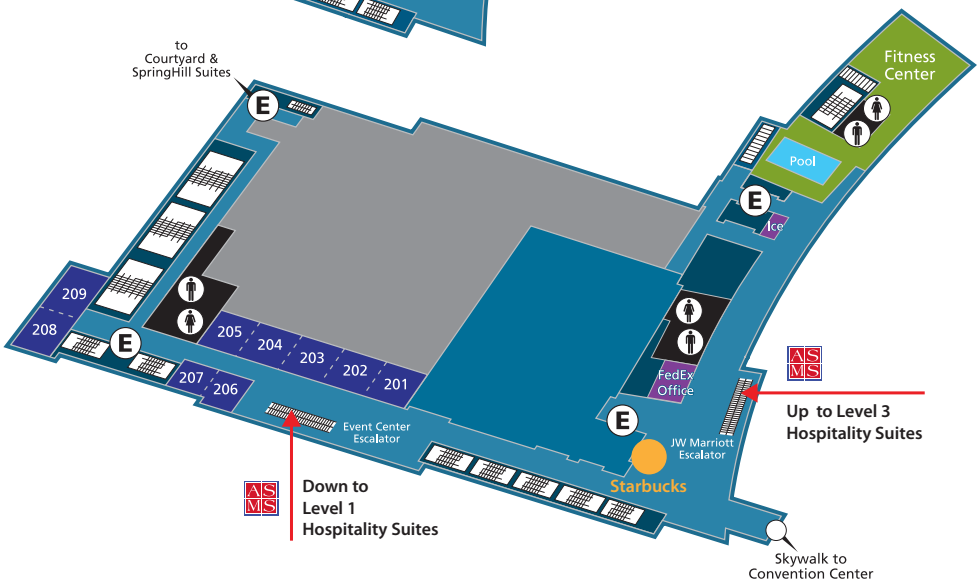


LEVEL 2

ESCALATORS
DOWN TO LEVEL 1
UP TO LEVEL 3

ACCESS to
COURTYARD & SPRINGHILL SUITES
SKYWALK to
CONVENTION CENTER
INDIANAPOLIS MARRIOTT

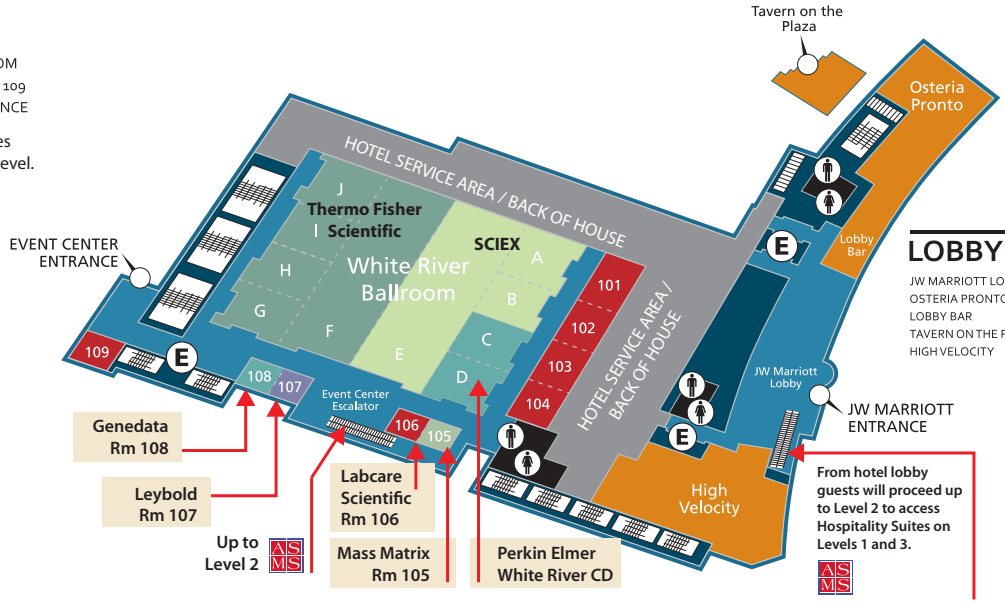
Level 2 serves as the access point to Hospitality Suites. From Level 2 guests can take escalators UP to Level 3 suites or down to Level 1 suites.



LEVEL 1

WHITE RIVER BALLROOM
MEETING ROOMS 101 - 109
EVENT CENTER ENTRANCE

Hospitality Suites located on this level.



BALLROOMS / EXHIBIT HALL
MEETING ROOMS
FITNESS CENTER / POOL
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Osteria Pronto
Lobby Bar
Tavern on the Plaza
High Velocity
T.G.I FRIDAY'S
SERVICES
FedEx Office
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Hertz Car Rental - (Level P1 at JW Marriott Garage Elevator)

ELEVATOR
RESTROOM - Men
RESTROOM - Women

LOBBY

JW MARRIOTT LOBBY
OSTERIA PRONTO
LOBBY BAR
TAVERN ON THE PLAZA
HIGH VELOCITY

HOSPITALITY SUITES 2017 - BACK TO BASICS

ASMS Corporate Member Hospitality Suites return to their roots in Indianapolis. When the hospitality suite concept was first introduced at the conference, the intention was to provide a relaxed atmosphere where attendees could interact with industry. To provide a setting for meaningful conversations regarding the latest technology in products and services, and attendees could network and enjoy refreshments.

In Indianapolis, hospitality suites will embrace the back to basics atmosphere which will allow attendees to learn more about Corporate Member products and services while enjoying fun, food, drink – and *conversation*.

Conference name badges are required for access to all conference activities including hospitality suites.

MEDIA EVENTS (PRESS CONFERENCES)

The following media events are scheduled **Monday, June 5** in the JW Marriott Hotel. All press are invited to attend these events.

8:00 - 9:00 am	Shimadzu Scientific Instruments	Grand Ballroom 5
9:30 - 10:30 am	Bruker Daltonics	Grand Ballroom 7-9
11:00 am - 12:00 pm	SCIEX	White River EAB
1:30 - 2:30 pm	Agilent Technologies	Grand Ballroom 6
3:00 - 4:00 pm	Thermo Fisher Scientific	White River F-J
4:30 - 5:30 pm	Waters Corporation	Grand Ballroom 1-4

BREAKFAST SEMINARS

Breakfast seminars are hosted by corporate members at either the Convention Center or the JW Marriott Hotel (inside hospitality suites). Pre-registration is recommended because room set-up and catering are arranged in advance. Please look for Breakfast Seminars page on www.asms.org and in the mobile app to find online registration links.

MONDAY BREAKFASTS	**CONVENTION CENTER**	*Start times vary, see below.*
	Advanced Chemistry Development	Room 140, 6:45 am
	LECO Corporation	Room 139, 6:45 am
	Matrix Science	Room 137-138, 7:00 am
	Perkin Elmer	Room 130, 7:00 am
	SCIEX (2)	Rooms 143-144 and 145, 7:00 am
	Shimadzu Scientific Instruments	Room 135-136, 7:00 am
	Waters Corporation	Room 133-134, 7:00 am
	JW MARRIOTT HOTEL	*Start times vary, see below.*
	Agilent Technologies	Grand Ballroom 6, 7:00 am
	Bruker Daltonics	Grand Ballroom 10, 7:00 am
	Thermo Fisher Scientific (2)	White River F and GH, 7:00 am
	Waters Corporation	Grand Ballroom 1-4, 7:00 am
TUESDAY BREAKFASTS	**CONVENTION CENTER**	*Start times vary, see below.*
	Biognosys	Room 130, 7:00 am
	LECO Corporation	Room 139, 6:45 am
	Matrix Science	Room 137-138, 7:00 am
	New Objective	Room 239, 6;45 am
	NIST Mass Spectrometry Data Center John Wiley and Sons Publishers	Room 141-142, 7:00 am
	Prosolia	Room 240, 7:00 am
	SCIEX (2)	Rooms 143-144 and 145, 7:00 am
	Shimadzu Scientific Instruments	Room 135-136, 7:00 am
	SYFT	Room 245, 7:00 am
	Waters Corporation	Room 133-134, 7:00 am
	JW MARRIOTT HOTEL	*Start times vary, see below.*
	Agilent Technologies	Grand Ballroom 6, 7:00 am
	Bruker Daltonics	Grand Ballroom 10, 7:00 am
	Thermo Fisher Scientific (2)	White River F and GH, 7:00 am
	Waters Corporation	Grand Ballroom 1-4, 7:00 am

WEDNESDAY BREAKFASTS	**CONVENTION CENTER**	*Start times vary, see below.*
	LECO Corporation	Room 139, 6:45 am
	New Objective	Room 130, 6:45 am
	SCIEX (3)	Rms 140, 143-144, and 145; 7:00 am
	Shimadzu Scientific Instruments	Room 135-136, 7:00 am
	JW MARRIOTT HOTEL	*Start times vary, see below.*
	Agilent Technologies	Grand Ballroom 6, 7:00 am
	Bruker Daltonics	Grand Ballroom 10, 7:00 am
	Thermo Fisher Scientific	White River F and GH, 7:00 am
	Waters Corporation	Grand Ballroom 1-4, 7:00 am
THURSDAY BREAKFASTS	**CONVENTION CENTER**	*Start times vary, see below.*
	SCIEX (2)	Rooms 143-144 and 145, 7:00 am
	Shimadzu Scientific Instruments	Room 135-136, 7:00 am
	Thermo Fisher Scientific	Room 141-142, 7:00 am

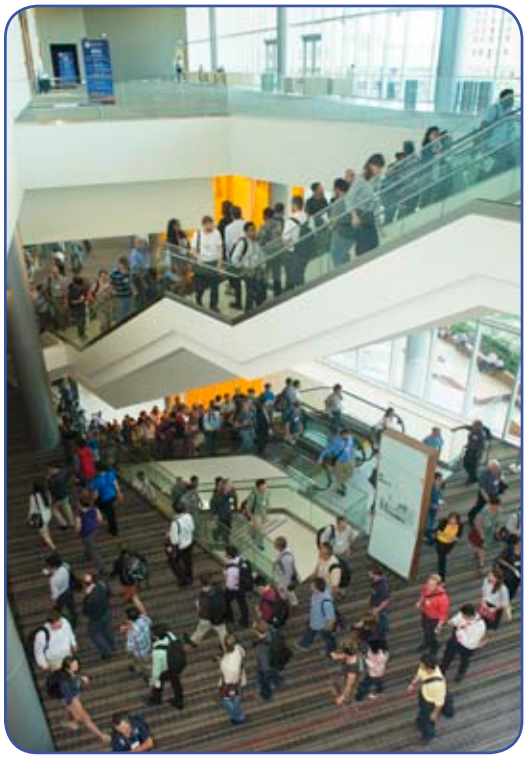
	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at JW Marriott	Breakfast Seminar
908 Devices	200			
AcroMass Technologies	729	Corporate Poster		
Advanced Chemistry Development (ACD/Labs)	711	Corporate Poster		Conv Ctr Rm 140: Mon 6/5
Advanced Chromotography Technologies, Ltd	101			
Advanced Energy	400	Corporate Poster		
Advion Inc.	506			
Agilent Technologies	600	Corporate Poster	Grand Ballroom 6	JW Marriott Grand 6: Mon-Wed (6/5-6/7)
American Chromatography Supplies	405			
Analytical Sales and Services, Inc.	605	Corporate Poster		
Anest Iwata	708			
Antec	519	Corporate Poster		
Apricot Designs, Inc.	303			
Ardara Technologies LP	324			
ASTA	421	Corporate Poster		
Avanti Polar Lipids, Inc.	928			
Baran Bioscience, LLC		Corporate Poster		
BioChromato, Inc.	821			
BIOCRATES Life Sciences AG	904			
Biognosys	507			Conv Ctr Rm 130: Tue 6/6
Bioinformatics Solutions Inc.	508	Corporate Poster		
Biopeptek, Inc	622			
Biotage	528			
Bonna-Agela Technologies, Inc.	227			
Bruker Daltonics	518		Grand Ballroom 7-10	JW Marriott Grand 10: Mon-Wed (6/5-6/7)
C&EN		Publisher Tabletop		
Cambridge Isotope Labs	618			
Cayman Chemical Company	803			
CDS Analytical	722			
CEM Corporation	619			
Cerno Bioscience	628			
Chemyx, Inc.	806			
CMP Scientific, Inc.	828			
Compare Networks		Publisher Tabletop		
CovalX	626			
CSS Analytical Co. Inc.	420			
CTC Analytics AG	607			
Detector Technology, Inc.	219			
Digital Proteomics	704			
Dikma Technologies, Inc	228			
Drummond Scientific	720			

	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at JW Marriott	Breakfast Seminar
EBARA Technologies	702			
Edwards Vacuum	707			
El-Mul Technologies	721			
e-MSion, Inc.	723			
Entech Instruments	918	Corporate Poster		
ESI Source Solutions	429			
ETP Electron Multipliers/Ion Detect	424	Corporate Poster		
Excellims Corporation	404			
Extrel	719			
Fasmatech	726			
FLIR Systems, Inc.	709			
Genedata	510	Corporate Poster	Room 108	
Genetic Engineering & Biotechnology News		Publisher Tabletop		
Genovis	706			
GenTech Scientific, Inc.	428			
GERSTEL, Inc.	524	Corporate Poster		
GL Sciences Inc.	401			
Grenova	724			
Hamamatsu Corporation	725			
Hamilton Company	810	Corporate Poster		
Harris Corp	418			
HILICON		Corporate Poster		
Horizon Technology, Inc.	727			
HTX Technologies, LLC	426			
IDEX Health & Science	411	Corporate Poster		
IMCS	201	Corporate Poster		
Imtakt USA	610			
InstruTech	224			
INTAVIS Bioanalytical Instruments AG	308			
Integrated Proteomics Applications	226			
International Ceramic Engineering	323			
International Equipment Trading Ltd.	504			
International Labmate		Publisher Tabletop		
Intertek Pharmaceutical Services	629			
ionBench	419			
Ionoptika Ltd	322			
IonSense, Inc.	718	Corporate Poster		
ION-TOF GmbH	425			
IsoSciences	203			
JASMS	111			
Jaytee Biosciences Ltd	302			
JEOL USA, Inc.	801			
Jordi Labs	423	Corporate Poster		
Kashiyama USA	804			

	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at JW Marriott	Breakfast Seminar
Knauer Wissenschaftliche Gerate GmbH	620			
Labcare Scientific International	205		Room 106	
Labcyte		Corporate Poster		
LECO Corporation	603	Corporate Poster		Conv Ctr Rm 139: Mon-Wed 6/5-6/7
Leybold USA Inc	525		Room 107	
Linden CMS GmbH	407			
MasCom Technologies	326			
MassMatrix		Corporate Poster	Room 105	
MassTech Inc.	327			
Matrix Science	328			Conv Ctr Rm 137-138: Mon 6/5, Tue 6/6
McKinley Scientific	606			
MeCour Temperature Control	229			
Mestrelab Research, S.L.	505			
MilliporeSigma	805			
Moeller Medical GmbH	521			
MPF Products Inc	210			
MRM Proteomics Inc	827			
MS Ekspert	320			
MS Noise	529			
MS Vision (Spectrometry Vision B.V.)	406			
mSPEC group	223			
MStm	705			
Nacalai USA, Inc.	829	Corporate Poster		
nanoLiter, LLC	209	Corporate Poster		
Navac LLC	808			
Nest Group, The		Corporate Poster		
New England Biolabs	908			
New England Peptide, Inc.	422			
New Objective, Inc.	604	Corporate Poster		Conv Ctr Rm 239: Tue 6/6, Conv Ctr Rm 130: Wed 6/7
NewOmics, Inc	809			
NIST	700			Conv Ctr Rm 141-142: Tue 6/6
Novilytic	609			
Omicron Biochemicals	509	Corporate Poster		
Omics, LLC	306	Corporate Poster		
Omni International	811			
Optimize Technologies, Inc.	403	Corporate Poster		
Owlstone Medical Ltd.	325			
Pace Analytical	119			
Parker Balston/Hannifin	409			
PEAK Scientific	701	Corporate Poster		

	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at JW Marriott	Breakfast Seminar
Perfinity Biosciences	523			
PerkinElmer	319		White River CD	Conv Ctr Rm 130: Mon 6/5
Pfeiffer Vacuum	301	Corporate Poster		
PharmaFluidics	225	Corporate Poster		
Phenomenex	627			
Phoenix S&T, Inc.	520			
PHOTONIS	300	Corporate Poster		
Physical Electronics	910	Corporate Poster		
Phytronix Technologies, Inc.	211			
Polymer Factory Sweden AB	310	Corporate Poster		
Postnova	608	Corporate Poster		
Presco Incorporated	202			
Pressure BioSciences, Inc.	329	Corporate Poster	Room 313	
Prolab Instruments GmbH	825			
Promega Corporation	800			
Prosolia, Inc.	611	Corporate Poster		Conv Ctr Rm 240: Tue 6/6
Protea Biosciences, Inc.	305			
Protein Metrics Inc.	410			
Proteome Software Inc.	218			
ProteoWorker	307	Corporate Poster		
Proton Onsite	621			
Prozyme, Inc.	427			
PURSPEC Technologies, Inc.	623			
Resolution Labs LLC	526			
Restek Corporation	900			
ReSyn Biosciences	408	Corporate Poster		
Samin Science Co., Ltd	129			
Science/AAAS		Publisher Tabletop		
Scientific Instrument Services	503	Corporate Poster		
Scientific Systems, Inc.	204			
SCIEX	500		White River EAB	Conv Ctr Rm 140: Wed 6/7 Conv Ctr Rm 143-144: Mon-Thur 6/5-6/8 Conv Ctr Rm 145: Mon-Thur 6/5-6/8
SepSolve Analytical	220			
Shimadzu Scientific Instruments, Inc.	511	Corporate Poster	Grand Ballroom 5	Conv Ctr Rm 135-136: Mon-Thur 6/5-6/8
Sierra Analytics	802	Corporate Poster		
Silantes GmbH	304			
SiO2 Medical Products	321		Room 314	
Sound Analytics	625			
Spark Holland	820			
SpectralWorks Limited	522	Corporate Poster		
Spectroscopy	822			
Spectroswiss	710			

Company	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at JW Marriott	Breakfast Seminar
Spellman High Voltage	818			
SPEX SamplePrep	207			
SunChrom GmbH	819			
Superior Technical Ceramics	221			
SYFT Technologies	402	Corporate Poster		Conv Ctr Rm 245: Tue, 6/6
The Analytical Scientist		Publisher Tabletop		
Thermo Fisher Scientific	601		White River F-J	Conv Ctr Rm 141-142: Thu 6/8 JW Marriott White River F & GH: Mon-Wed 6/5-6/7
Tofwerk AG	624			
Tosoh Bioscience	728			
Trajan Scientific and Medical	703	Corporate Poster		
Veritomyx	318	Corporate Poster	Room 313	
VICI Valco Instruments	824			
VRS	602			
VUV Analytics	311			
Waters Corporation	501	Corporate Poster	Grand Ballroom 1-4	Conv Ctr Rm 133-134: Mon-Tues 6/5-6/6 JW Marriott Grand 1-4: Mon-Wed 6/5-6/7
Wiley		Publisher Tabletop		Conv Ctr Rm 141-142: Tue 6/6
XPC Corporation	502			
Zef Scientific Inc.	309			
Zhejiang Haochuang Biotech Co., Ltd	826			



Vice President for Programs

Richard A. Yost
University of Florida
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.

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Marc Engel	Skip Kingston	Matt Schenauer	
Kenyon M. Evans-Nguyen	M. Violet Lee	David Schroeder	
	Cheng Lin	Salvatore Sechi	

SATURDAY

9:00 AM - 4:30 PM	**Short Courses**
2:00 - 5:00 PM	**Registration**

SUNDAY

9:00 AM - 4:30 PM	**Short Courses**
10:00 AM - 8:00 PM	**Registration**
4:00 - 4:45 PM	**Attention: First-time Graduate Students and Undergraduate Students** **Plan your Strategy: What to See and Do at ASMS,** Room 107-110 level 1
5:00 - 6:30 PM	**Tutorial Lectures,** Hall D level 1 **5:00 - 5:45 pm** **MALDI: Past and Future** **Kermit K. Murray,** *Louisiana State University*  **5:45 - 6:30 pm** **Cancer Immunotherapy and Mass Spectrometry** **Donald F. Hunt,** *University of Virginia*  **Tutorial Session II,** Wabash level 1 **5:00 - 5:45 pm** **Ion Mobility Spectromety: Analyzing Molecules as They Tumble through Life** **Erin S. Baker,** *Pacific Northwest National Lab*  **5:45 - 6:30 pm** **CE/MS -Ready for Prime Time?** **Norman J. Dovichi,** *University of Notre Dame* 
6:45 - 7:45 PM	**Conference Opening,** Hall D level 1 **Richard A. Yost,** *University of Florida* *ASMS Vice President for Programs*  **7:00 - 7:45 pm** **Towards a Good Start in Life: Neonatal Screening and Beyond** **David S. Millington** *Duke University Medical Center*
7:45 - 9:00 PM	**Welcome Reception in the Poster/Exhibit Hall** Undergraduate Student Poster Competition

MONDAY

From 6:45 AM	**Corporate Breakfast Seminars,** Convention Center and JW Marriott Hotel (schedule on page 15)
7:30 AM - 5:00 PM	**Registration**
8:30 - 10:30 AM	**Oral Sessions** MOA am: Celebration of Klaus Biemann's Science, *Hall D level 1* MOB am: Applications of Stable Isotope Labeling in MS, *500 Ballroom level 1* MOC am: Metabolomics: New Technologies and Applications, *Sagamore 1-3 level 2* MOD am: Innovations and Applications in Forensics, *Sagamore 4 level 2* MOE am: Plant "omics", *Sagamore 5-7 level 2* MOF am: Ion Mobility: New Developments and Applications, *Wabash level 1* MOG am: Instrumentation: New Developments in Ion Detection, *Room 101-106 level 1* MOH am: Synthetic Polymers, *Room 107-110 level 1*
10:30 AM - 2:30 PM	**Poster Session and Exhibits,** Monday Posters, Poster/Exhibit 11:30 am - 1:00 pm: **Undergraduate students** – look for reserved tables and free lunch vouchers to ***Meet the Experts***
2:30 - 4:30 PM	**Oral Sessions** MOA pm: MS in Clinical Analysis, *Hall D level 1* MOB pm: Analytical Challenges of Microdosing and Microsampling Studies, *500 Ballroom level 1* MOC pm: Metabolomics: Untargeted Profiling, *Sagamore 1-3 level 2* MOD pm: Environmental: Emerging Contaminants, *Sagamore 4 level 2* MOE pm: Hydrogen-Deuterium Exchange MS, *Sagamore 5-7 level 2* MOF pm: Ion Mobility: Small Molecules, Pharmaceuticals, and DMPK, *Wabash level 1* MOG pm: Instrumentation: Ambient Ionization: Instrumentation & Applications, *Rm 101-106 level 1* MOH pm: Fundamentals: Ion-Ion and Ion-Neutral Interactions, *Room 107-110 level 1*
4:45 - 5:30 PM	**Award Lecture**, Hall D level 1 **Award for a Distinguished Contribution in Mass Spectrometry**  **Catherine E. Costello** *Boston University*
5:45 - 7:00 PM	**Workshops** There are light refreshments in the common areas. 01. Improving Scientific Writing Skills, *Room 130 level 1* 02. Metal Ion Coordination in Gas-Phase Bioanalysis: Reaping Practical Benefits (Metal Ion Coordination Chemistry Interest Group), *Room 131-132 level 1* 03. Open Source Software Packages: Using and Making your Contributions (Bioinformatics MS Interest Group), *Room 133-134 level 1* 04. Clinical Diagnostics: Translating New Mass 8. Spectrometry Approaches (Clinical Chemistry Interest Group), *Room 135-136 level 1* 05. FTMS: Successes and Challenges of Achieving Routinely High Mass Accuracy (FTMS Interest Group), *Room 137-138 level 1* 06. Exposomics Update: Success, Lessons and Future Goals (Exposomics Interest Group), *Room 139 level 1* 08. Antibody-Drug Conjugate Research and Development: The Role of Multifaceted Mass Spectrometry (Pharmaceuticals Interest Group), *Room 141-142 level 1* 09. Forensics and Homeland Security Mass Spectrometry Research: A Critical Discussion between Academicians and Forensic Science Practitioners (Forensics & Homeland Security Interest Group), *Room 143-144 level 1* 10. Art and Cultural Heritage: Mass Spec Applications, *Room 145 level 1* 11. Mass Spectrometry Interactive Virtual Environment (MassIVE): Management of Big Data, *Room 231-234 level 2* 12. Ion Trap Instrumentation for Harsh Environment and Point-of-Care Applications (Ion Trap MS Interest Group), *Room 235-238 level 2* 13. Photoionization: Applications, Developments, and Discussions (Photoionization MS Interest Group), *Room 239 level 2* 14. A Career in Mass Spec: Options and Where to start? (Young Mass Spectrometrists Interest Group), *Room 240-242 level 2* 15. Top-Down Proteomics, *Room 243-245 level 2*
7:00 - 8:00 PM	**Dinner Break**
After 8:00 PM	**Corporate Hospitality Suites,** JW Marriott Hotel

TUESDAY

From 6:45 AM	**Corporate Breakfast Seminars,** Convention Center and JW Marriott Hotel (schedule on page 15)
7:30 AM - 5:00 PM	**Registration**
8:30 - 10:30 AM	**Oral Sessions** TOA am: Informatics: Peptide and Protein Identification, *Hall D level 1* TOB am: Quantitative Analysis in Drug Discovery and Development, *500 Ballroom level 1* TOC am: Qualitative and Quantitative Analysis of PTMs, *Sagamore 1-3 level 2* TOD am: Exposomics: Targeted, Untargeted and Bioinformatics Methodologies, *Sagamore 4 level 2* TOE am: Macromolecular Complexes, *Sagamore 5-7 level 2* TOF am: Ion Mobility: Structure, *Wabash level 1* TOG am: Instrumentation: Mass Analyzer Innovations, *Room 101-106 level 1* TOH am: Fundamentals: Ion Spectroscopy, *Room 107-110 level 1*
10:30 AM - 2:30 PM	**Poster Session and Exhibits,** Tuesday Posters, Poster/Exhibit Hall
2:30 - 4:30 PM	**Oral Sessions** TOA pm: Informatics: Metabolomics, *Hall D level 1* TOB pm: MS in the Regulatory Environment, *500 Ballroom level 1* TOC pm: Quantitative Proteomics in Systems Biology, *Sagamore 1-3 level 2* TOD pm: Environmental: New Instrumentation and Approaches, *Sagamore 4 level 2* TOE pm: Covalent Labeling and Chemical Crosslinking, *Sagamore 5-7 level 2* TOF pm: Microorganisms: Identification and Characterization, *Wabash level 1* TOG pm: Instrumentation: Innovations in FT-based Mass Analyzers, *Room 101-106 level 1* TOH pm: Fundamentals: Ion Activation and Dissociation, *Room 107-110 level 1*
4:45 - 5:30 PM	**Award Lecture,** Hall D level 1 **Biemann Medal**  **Ryan Julian** *University of California, Riverside*
5:45 - 7:00 PM	**Workshops** There are light refreshments in the common areas. 01. Trans-Proteomic Pipeline: New Advances and Future Developments, *Room 130 level 1* 02. Bioinformatic Approaches for Glycomics/ Glycoproteomics, *Room 131-132 level 1* 03. Statistics and Bioinformatics using R, *Room 133-134 level 1* 04. Environmental Analysis: Modern Sampling Techniques and Data Analysis (Environmental Applications Interest Group), *Room 135-136 level 1* 05. Hepatocytes: Current and Future Use in DMPK (DMPK Interest Group), *Room 137-138 level 1* 06. The NIH and NSF Review and Funding Process, *Room 139 level 1* 07. Proteomic Workflow: Unpublished Collective Practical Knowledge from Insiders (Analytical Lab Managers Interest Group), *Room 140 level 1* 08. The Need for Speed: Is your LC or Mass Spectrometer the Top Gun for Improving Throughput? (LCMS & Related Topics Interest Group), *Room 141-142 level 1* 09. Tracing Uncertainty in Imaging MS: Benchmarking Reproducibility, Variability, and Performance across Experiments (Imaging MS Interest Group), *Room 143-144 level 1* 10. JASMS - Present Status and Future, *Room 145 level 1* 11. Biotherapeutics: Hot Topics (Biotherapeutics Interest Group), *Room 231-234 level 2* 12. HDX, Covalent Labeling & Cross Linking: State-of-the-Art and Future Directions (HDX Covalent Labeling & Cross Linking Interest Group), *Room 235-238 level 2* 13. Polymer Mass Spectrometry: Advances (Polymeric Materials Interest Group), *Room 239 level 2* 14. Metabolomics: Integration into the Emerging Arena of Multi-omic Approaches (Metabolomics Interest Group), *Room 240-242 level 2* 15. Mass Spectrometry and Ion Mobility: The Role of Temperature (Fundamentals Interest Group), *Room 243-245 level 2*
7:00 - 8:00 PM	**Dinner Break**
After 8:00 PM	**Corporate Hospitality Suites,** JW Marriott Hotel

WEDNESDAY

From 6:45 AM	**Corporate Breakfast Seminars,** Convention Center and JW Marriott Hotel (schedule on page 15)
7:30 AM - 5:00 PM	**Registration**
8:30 - 10:30 AM	**Oral Sessions** WOA am: Informatics: DIA: Innovative Methods and Applications, *Hall D level 1* WOB am: Food Safety & Chemistry: Non-targeted Screening, *500 Ballroom level 1* WOC am: Biomarkers: Qualitative Analysis, *Sagamore 1-3 level 2* WOD am: Lipidomics: Lipids and Profiling, *Sagamore 4 level 2* WOE am: Glycopeptides and Glycoproteins, *Sagamore 5-7 level 2* WOF am: Imaging: Instrumentation & Method Development, *Wabash level 1* WOG am: Instrumentation: MS in Extreme Environments, *Room 101-106 level 1* WOH am: Fundamentals: Photoionization and Photodissociation, *Room 107-110 level 1*
10:30 AM - 2:30 PM	**Poster Session and Exhibits,** Wednesday Posters, Poster/Exhibit Hall
2:30 - 4:30 PM	**Oral Sessions** WOA pm: Informatics: Multiomics Integration and Applications, *Hall D level 1* WOB pm: Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, *500 Ballroom level 1* WOC pm: Antibodies and Antibody Drug Conjugates, *Sagamore 1-3 level 2* WOD pm: Lipidomics: New MS Technologies and Applications, *Sagamore 4 level 2* WOE pm: Biomarkers: Quantitative Analysis, *Sagamore 5-7 level 2* WOF pm: Imaging: Computational Methods and Analysis, *Wabash level 1* WOG pm: Instrumentation: New Developments in Ionization and Sampling, *Room 101-106 level 1* WOH pm: Fundamentals: Molecular Modeling and Quantum Mechanical Calculations in Ion Mobility and MS, *Room 107-110 level 1*
4:45 - 5:30 PM	**ASMS Meeting,** Sagamore 5-7 level 2: Awards, board reports, wine, beer, soft drinks - and more!
5:45 - 7:00 PM	**Workshops** There are light refreshments in the common areas. 01. Career and Collaboration Opportunities in China, *Room 130 level 1* 02. High Spatial Resolution 2D and 3D Mass Spectrometry Analysis: New Trends, *Room 131-132 level 1* 03. Diversity and Outreach, *Room 133-134 level 1* 04. Galaxy-P in the Cloud: Proteomic Informatics on JetStream, *Room 135-136 level 1* 05. Food Safety & Authenticity: HRMS Applications (Flavor, Fragrance & Foodstuff Interest Group), *Room 137-138 level 1* 06. Energy, Petroleum, and Biofuels: Experimental Challenges (Energy Petroleum & Biofuels Interest Group), *Room 139 level 1* 07. Undergraduate Research in Mass Spectrometry: Making the Most of It (Undergraduate Research in MS Interest Group), *Room 140 level 1* 08. Quantitative Glycomics and Glycoproteomics, *Room 141-142 level 1* 09. Mass Spectrometry in GMP Environment: Aspects of System Qualification and Method Validation, *Room 143-144 level 1* 10. Mass Spectrometry in the Developing World: Supporting Education and Research, *Room 145 level 1* 11. Lipidomics Data Processing and Analyses: Software Tools (Lipids & Lipodomics Interest Group), *Room 231-234 level 2* 12. Data Independent Acquisition Strategies for Quantitative Proteomics: The Challenges of Scaling Up to Meet Demand (Data Independent Acquisition Interest Group), *Room 235-238 level 2* 13. Nucleic Acid-based Therapeutics: Structure Identification and Bioanalysis (Oligonucleotides and Nucleic Acids Interest Group), *Room 239 level 2* 14. Ion Mobility Spectrometry: Towards Standard Operating Procedures (Ion Mobility MS Interest Group), *Room 240-242 level 2* 15. Bioanalysis of Biosimilars (Regulated Bioanalysis Interest Group), *Room 243-245 level 2*
7:00 - 8:00 PM	**Dinner Break**
After 8:00 PM	**Corporate Hospitality Suites,** JW Marriott Hotel

THURSDAY

From 6:45 AM	**Corporate Breakfast Seminars,** Convention Center (schedule on page 15)
7:30 AM - 5:00 PM	**Registration**
8:30 - 10:30 AM	**Oral Sessions** ThOA am: Informatics: Innovations, *Hall D level 1* ThOB am: MS in the QC Lab, *500 Ballroom level 1* ThOC am: Membrane Protein MS, *Sagamore 1-3 level 2* ThOD am: Nucleic Acids and Oligonucleotides, *Sagamore 4 level 2* ThOE am: Native MS in Structural Biology, *Sagamore 5-7 level 2* ThOF am: Imaging: Pharmaceuticals, Metabolites, and Lipids, *Wabash level 1* ThOG am: GC/MS, GC/GC/MS, GC/MS/MS, and GC/HRMS, *Room 101-106 level 1* ThOH am: Fundamentals for Everyone, *Room 107-110 level 1*
10:30 AM - 2:30 PM	**Poster Session and Exhibits,** Thursday Posters, Poster/Exhibit Hall
2:30 - 4:30 PM	**Oral Sessions** ThOA pm: Informatics: Discovery Proteomics, *Hall D level 1* ThOB pm: HRMS for Quantitation in Drug Discovery, Development & Beyond, *500 Ballroom level 1* ThOC pm: Top Down Protein Analysis, *Sagamore 1-3 level 2* ThOD pm: Carbohydrates, *Sagamore 4 level 2* ThOE pm: Protein-Ligand Interactions, *Sagamore 5-7 level 2* ThOF pm: Imaging: Biomedical Applications, *Wabash level 1* ThOG pm: Instrumentation: Separations Approaches Coupled to MS, *Room 101-106 level 1* ThOH pm: Energy, Petroleum, and Biofuels: Instrumentation & Applications, *Room 107-110 level 1*
4:45 - 5:30 PM	**Plenary Lecture,** Hall D level 1  **Saving the Great Coral Reefs** **Kristen Marhaver** *Research Station Carmabi*
6:30 - 9:00 PM	**Closing Event at the Indiana State Museum** Advance purchase ticket required. The museum is located in the park-like area behind the JW Marriott Hotel complex, an easy walk from convention center and downtown hotels.

SUNDAY EVENING, 4:00 - 9:00 PM

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 (Grinnell College) and
JC Poutsma (College of William & Mary)
Room 107-110 level 1

5:00-6:30 pm Sunday
TUTORIAL SESSION I
Richard A. Yost (University of Florida)
Hall D level 1

5:00-5:45 pm
MALDI: Past and Future
Kermit K. Murray
Louisiana State University

5:45-6:30 pm
Cancer Immunotherapy and Mass Spectrometry
Donald F. Hunt
University of Virginia

5:00-6:30 pm Sunday
TUTORIAL SESSION II
John A. McLean (Vanderbilt University)
Wabash level 1

5:00-5:45 pm
Ion Mobility Spectrometry: Analyzing Molecules as They Tumble through Life
Erin S. Baker
Pacific Northwest National Laboratory

5:45- 6:30 pm
CE/MS - Ready for Prime Time?
Norman J. Dovichi
University of Notre Dame

6:45-7:45 pm Sunday
Conference Opening
Richard A. Yost (University of Florida)
Hall D level 1

Welcome, Richard A. Yost, *University of Florida*
ASMS Vice President for Programs

7:00-7:45 pm
Towards a Good Start in Life: Neonatal Screening and Beyond
David S. Millington
Duke University Medical Center

7:45-9:00 pm Sunday
WELCOME RECEPTION
Poster/Exhibit Hall
Conference name badge is required.

MONDAY MORNING ORAL SESSIONS

From 6:45 am Monday
CORPORATE BREAKFAST SEMINARS
Convention Center and JW Marriott Hotel
Detailed schedule on page 15.
Pre-registration recommended, space is limited

8:30-10:30 am Monday
CELEBRATION OF KLAUS BIEMANN'S SCIENCE
Dominic Desiderio (Univ. of Tennessee Health Science)
Hall D level 1

MOA am 08:30 **A Son's Perspectives on Klaus Biemann's Life**; Hans-Peter Biemann; *Sanofi Genzyme, Cambridge, MA*

MOA am 08:50 **Who Invented GC/MS?** Ronald A. Hites; *Indiana University, Bloomington, IN*

MOA am 09:10 **Identification of Tumor Specific, Class I MHC Peptides for Immunotherapy of Cancer: Instrumentation and Methods for Characterization of Intact Proteins**; Donald F. Hunt; *University of Virginia, Charlottesville, VA*

MOA am 09:30 **A Career of Lipid Biochemistry and Mass Spectrometry: From Fatty Acids to Lipidomics**; Robert C. Murphy; *Univ of Colorado Denver, Aurora, CO*

MOA am 09:50 **New Approaches for Localization of Proteins and Interaction Partners in Cells with High Spatial Resolution**; Steven A. Carr; *Broad Institute, Cambridge, MA*

MOA am 10:10 **CSI@MIT: Adventures in the Biemann Laboratory**; Catherine E. Costello; *Boston University School of Medicine, Boston, MA*

8:30-10:30 am Monday
APPLICATIONS OF STABLE ISOTOPE LABELING IN MS
Teresa Fan (University of Kentucky)
500 Ballroom level 1

MOB am 08:30 **Unveiling Metabolic Origins of Cell Surface Glycosylation and Turnover Kinetics of Glycoproteins Using 13C-labeled Saccharides and LC-MS/MS Analysis**; Gege Xu[1]; Maurice Wong[1]; Qiongyu Li[1]; Mariana Barboza[1]; Dayoung Park[1]; Zhi Cheng[1]; Carlito B. Lebrilla[1]; *[1]University of California, Davis, Davis, California*

MOB am 08:50 **Turnover Measurements of Low Abundance Proteins in Human Plasma and PBMCs by Serial Immunoaffinity and Mass Spectrometry**; Vahid Farrokhi[1]; Teresa Caiazzo[1]; Katherine Wright[1]; Dnise O'Hara[1]; Hendrik Neubert[1]; *[1]Pfizer, Inc., Andover, MA*

MOB am 09:10 **Influence of the Gut Microbiota on Histone Modifications in Intestinal Epithelial Cells**; Peder J. Lund[1]; Sarah A. Smith[2]; Johayra Simithy[1]; Zuo-Fei Yuan[1]; Kevin A. Janssen[1]; Gary D. Wu[2]; Benjamin A. Garcia[1]; *[1]Penn Epigenetics Institute, Dept. of Biochemistry and Biophysics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA; [2]Dept. of Medicine, Division of Gastroenterology, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA*

MOB am 09:30 **Metabolic Tracing in Hepatocytes Demonstrates the Contribution of acetyl-CoA Derived from Ethanol Metabolism to Histone Acetylation**; Crystina Kriss[1]; Stanley M Stevens Jr[2]; *[1]University of South Florida, Tampa, FL; [2]University of South Florida, Tampa, FL*

MOB am 09:50 **Quantitative *in vitro* Proteomic Profiling of Colon Cancer Spheroids treated with Combination Chemotherapy in a 3D printed Fluidic Device**; Gabriel LaBonia[1]; Amanda B. Hummon[1]; *[1]University of Notre Dame, Notre Dame, IN*

MOB am 10:10 **Resolution of 13C and Deuterium Isotopes Allows Lipid Fluxomics Analysis By Rate of Deuterium Incorporation**; Matthew Mitsche[1]; Goncalo Vale[1]; Jeffrey McDonald[1]; *[1]University of Texas Southwestern Medical Center, Dallas, TX*

8:30-10:30 am Monday
METABOLOMICS: NEW TECHNOLOGIES AND APPLICATIONS
Leah Shriver (University of Akron)
Sagamore 1-3 level 2

MOC am 08:30 **A Metabo-Redoxome Platform for Comprehensive Survey of Oxidative Stress Severity in the Lower Respiratory Tract of Smokers and HIV-infected Subjects**; Miriam Sindelar[1]; Sarah L O'Beirne[1]; Philip L Leopold[1]; Michelle R Staudt[1]; Robert J Kaner[1]; Ronald G Crystal[1]; Steven S Gross[1]; *[1]Weill Cornell Medicine, New York, NY*

MOC am 08:50 **Stable Isotope-Resolved Metabolomic (SIRM) Studies of *in vitro*, *in vivo*, and *ex vivo* Isogenic Human Cancer Models Using Ion-Chromatography MS**; Marc O. Warmoes[1]; Qiushi Sun[1]; Ramon Sun[1]; Penghui Lin[1]; Andrew N. Lane[1]; Richard M. Higashi[1]; Teresa W.-M. Fan[1]; *[1]University of Kentucky, Lexington, KY*

MOC am 09:10 **Differentiation of Acylcarnitine Isomers Based on LC-MS/MS Mass Spectra and Development of an Accurate Mass Spectral Library**; Xinjian Yan[1]; Yuri Mirokhin[1]; Ramesh Marupaka[1]; Yamil Simón-Manso[1]; Dmitrii Tchekhovskoi[1]; Stephen E Stein[1]; *[1]NIST, Gaithersburg, MD*

MOC am 09:30 **Microprobe Single-cell CE-ESI-MS Captures Metabolic Changes in the Developing Frog (Xenopus laevis)Embryo**; Rosemary Masu Onjiko[1]; Erika P Portero[1]; Sally A Moody[1]; Peter Nemes[1]; *[1]George Washington University , Washington, DC*

MOC am 09:50 **Solid Phase Microextraction: A New Tool for *in vivo* monitoring of Metabolic Changes Occurring During Deep Brain Stimulation**; Nathaly Reyes Garces[1]; Ezel Boyacı[1]; German A. Gomez-Rios[1]; Barbara Bojko[1, 2]; Clement Hamani[3]; Janusz Pawliszyn[1]; *[1]University of Waterloo, Waterloo, ON, Canada; [2]Nicolaus Copernicus University in Torun, Bydgoszcz, Poland; [3]University of Toronto, Toronto, ON, Canada*

MOC am 10:10 **FAC-MS: A New Platform Coupling Heterologous Expression and Untargeted Metabolomics for Large-Scale Fungal Natural Product Discovery**; Ken Clevenger[1]; Jinwoo Bok[2]; Rosa Ye[3]; Galen P Miley[4]; Maria H Verdan[4]; Thomas Velk[2]; Cynthia Chen[3]; KaHoua Yang[2]; Matthew Robey[4]; Peng Gao[4]; Matthew Lamprecht[3]; Md Nurul Islam[3]; Jonathan Palmer[5]; PAUL Thomas[4]; ChengCang Wu[3]; Nancy Keller[2]; Neil L Kelleher[4]; *[1]Northwestern University, Evanston, IL; [2]University of Wisconsin Madison, Madison, WI; [3]Intact Genomics, St. Louis, MO; [4]Northwestern University, Evanston, IL; [5]US Forest Service, Madison, WI*

8:30-10:30 am Monday
INNOVATIONS AND APPLICATIONS IN FORENSICS
Marilyn Tourne (Tuskegee University)
Sagamore 4 level 2

MOD am 08:30 **Paper Spray Mass Spectrometry for the Detection of Chemical Warfare Agent Simulants**; Elizabeth S Dhummakupt[1, 2]; Josiah McKenna[3]; Theresa Connell[4]; Paul Demond[4]; Dennis B Miller[1]; Nicholas E Manicke[3]; J Michael Nilles[4]; Trevor Glaros[1]; *[1]US Army ECBC, Aberdeen Proving Ground, MD; [2]National Research Council, Washington, DC; [3]Indiana University-Purdue University Indianapolis, Indianapolis, IN; [4]Excet, Inc., Springfield, VA*

MOD am 08:50 **Development of a High Sensitivity Method for Direct Characterisation of Forensic Samples**; Efstathios Elia[1]; Samantha Leach[2]; I-Chung Lu[1]; Milan Pophristic[3]; Sarah Trimpin[1]; *[1]Wayne State University, Detroit, MI; [2]DC Department of Forensic Sciences (DFS), Washington, DC; [3]MSTM, LLC., Newark, DE*

MOD am 09:10 **Rapid Absolute Quantification of Abrin Toxin and Its Isoforms in Complex Matrices by Immuno-extraction and High Resolution Targeted Mass Spectrometry**; Eva-Maria Hansbauer[1]; Sylvia Worbs[2]; François Fenaille[1]; Hervé Volland[3]; Stéphanie Simon[3]; Christophe Junot[1]; Brigitte G. Dorner[2]; François Becher[1]; *[1]CEA Saclay, DRF, iBiTec-S, Service de Pharmacologie et d'Immunoanalyse, Laboratoire d'Etude du Métabolisme des Médicaments, Gif-sur-Yvette, France; [2]Biological Toxins, Centre for Biological Threats and Special Pathogens, Robert Koch Institute, Berlin, Germany; [3]CEA Saclay, DRF, iBiTec-S, Service de Pharmacologie et d'Immunoanalyse, Laboratoire d'Etudes et de Recherches en Immunoanalyse, Gif-sur-Yvette, France*

MOD am 09:30 **Identification of Fentanyl and Other Synthetic Opiates using Ambient Ionization High Resolution Time-of-Flight Mass Spectrometry**; Jamie Foss[1]; Amanda Moore[2]; Sabra Botch-Jones[2]; Maria Pease[3]; Frank Kero[4]; *[1]PerkinElmer, Shelton , CT; [2]Boston University School of Medicine, Boston, MA; [3]Maine Health and Environmental Testing Laboratory, Augusta, ME; [4]PerkinElmer, Downers Grove, IL*

MOD am 09:50 **Development of Solid Phase Microextraction (SPME) Devices for Analysis of Drugs in Biofluids via Direct Analysis in Real Time (DART)**; Tijana Vasiljevic[1]; German Augusto Gomez-Rios[1]; Emanuela Gionfriddo[1]; Janusz Pawliszyn[1]; *[1]University of Waterloo, Waterloo, ON, Canada*

MOD am 10:10 **Isomeric Separation of Cannabinoids by UPLC-ESI(±)TWIM-MS**; Lilian V. Tose[1]; Samantha R.C. Silva[1]; Michael Murgu[2]; Boniek Gontijo Vaz[3, 4]; Wanderson Romão[4, 5]; *[1]Federal University of Espírito Santo, Vitória, Brazil; [2]Waters Corporation, São Paulo, Brazil; [3]Federal University of Goiás, Goiânia, GO; [4]National Institute of Forensic Science and Technology (INCT), Vila Velha, Brazil; [5]IFES/UFES, Vila Velha, Brazil*

8:30-10:30 am Monday
PLANT "OMICS"
Erin Gemperline (Dow Agrosciences)
Sagamore 5-7 level 2

MOE am 08:30 **Plant Ionomics Profiling: Development of a High-throughput Multi-elemental Profiling Technique Using ICP-MS and Case Studies in Onion, Potato and Barley**; Jacqueline M. Chaparro[1, 2]; Corey D. Broeckling[1]; Jessica E. Prenni[1]; Adam L. Heuberger[2]; *[1]Colorado State University's Proteomics and Metabolomics Facility, Fort Collins, CO; [2]Colorado State University Department of Horticulture and Landscape Architecture, Fort Collins, CO*

MOE am 08:50 **Direct Identification of Mosaic Virus Induced Molecular Signature Changes in Plant Leaves Using High Throughput Laser-REIMS Technology**; Richard Schäffer[1]; Julia Balog[2, 3]; Gabriel Horkovics-Kovats[2]; Tamas Karancsi[2]; Steven Derek Pringle[3, 4]; Katalin Salánki[5]; Ákos Gellért[5]; Zoltan Takats[3]; *[1]Waters Research Center, Budapest; [2]Waters Research Center, Budapest; [3]Imperial College London, London; [4]Waters Corporation, Wilmslow, UK; [5]Centre for Agricultural Research, Hungarian Academy of Sciences, Budapest, Hungary*

MOE am 09:10 **Implementation of a Spatial Metabolomics Approach for Exploring Interactions within a Tripartite Plant-Fungus-*cyanobacterium* System**; Dusan Velickovic[1]; Alyssa A. Carrell[2]; Rosalie K. Chu[1]; Malak M. Tfaily[1]; Dale Pelletier[3]; Samuel M. D. Seaver[4]; Mathew Thomas[1]; Ljiljana Pasa-Tolic[1]; David J. Weston[2, 3]; Christopher R Anderton[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Department of Biology, Duke University, Durham, NC; [3]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN; [4]Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL*

MOE am 09:30 **Proteomic Profiling to Identify the Unintended Effects of Genetic Modification on Gluten Proteins**; Sophie Bromilow[1]; Lee A Gethings[2]; Mike Buckley[3]; Peter Shewry[4]; E. N. C Mills[1]; *[1]School of Biological Science, Manchester Institute of Biotechnology, Manchester, UK; [2]Waters Corporation, Wilmslow, UK; [3]School of Environmental Sciences, Manchester Institute of Biotechnology, Manchester, UK; [4]Rothamsted Research, Harpenden, UK*

MOE am 09:50 **Large Scale Integration of Proteomics and Genomics Data to Enhance Rice Genome Annotation**; Da Qi[1]; Zhe Ren[2]; Bo Wen[2]; Ruo Zhou[2]; Siqi Liu[2, 3]; Andrew R Jones[1]; *[1]University of Liverpool, Liverpool, UK; [2]The BGI-Shenzhen, Shenzhen, China; [3]Beijing Institute of Genomics, Chinese Academy of Sciences, Beijing, China*

MOE am 10:10 **Streamlining Phosphoproteomic Workflow to Study Plant Signaling and Its Application to Tomato Phosphoproteomics**; Chuan-Chih Hsu[1]; Yingfang Zhu[1]; Pengcheng Wang[1]; Peipei Zhu[1]; I-Hsuan Chen[1]; Yuan Zhou[1]; Jian-Kang Zhu[1]; Andy Tao[1]; *[1]Purdue University, West Lafayette, IN*

8:30-10:30 am Monday
ION MOBILITY: NEW DEVELOPMENTS & APPLICATIONS
Theresa Evans-Nguyen (Univ. of Southern Florida)
Wabash level 1

MOF am 08:30 **A New Instrument with High Mass and High Ion Mobility Resolution**; Michael T. Bowers [1]; Thomas Wyttenbach[2]; Paul R Kemper[2]; Mel Park[3]; Goekhan Baykut[4]; *[1]University of California, Santa Barbara , CA; [2]University of California Santa Barbara, Santa Barbara, CA; [3]Bruker Daltonics, Billerica, MA; [4]Bruker Daltonik GmbH, Bremen, Germany*

MOF am 08:50 **Discovery and Targeted Monitoring of *D. discoideum* Lipids using Multidimensional LC-TIMS-MS/MS Separations**; Kendra J. Adams[1]; Cesar E. Ramirez[1]; Richard H. Gomer[2]; Francisco Fernandez-Lima[1, 3]; *[1]Florida International University, Miami, FL; [2]Texas A&M University, College Station, Texas; [3]Biomolecular Sciences Institute, Miami, FL*

MOF am 09:10 **Conformationally Dependent Peptide Hydrolysis Measured by Temperature Controlled ESI-IMS-MS**; Daniel R. Fuller[1]; Christopher R. Conant[1]; Tarick J. El-Baba[2]; Zhichao Zhang[2]; Daniel W. Woodall[2]; David H. Russell[3]; David E. Clemmer[2]; *[1]Indiana University Bloomington, Bloomington, IN; [2]Indiana University Bloomington, Bloomington, IN; [3]Texas A&M University, College Station, TX*

MOF am 09:30 **Multidimensional, Time-resolved Trapped Ion Mobility Spectrometry-Mass Spectrometry (TIMS/TIMS-MS) to Elucidate Conformations of Proteins**; Fanny Caroline Liu[1]; Mark E Ridgeway[2]; Melvin A Park[2]; Christian Bleiholder[1]; *[1]Florida State University, Tallahassee, FL; [2]Bruker Daltonics, Billerica, MA*

MOF am 09:50 **Transformational Approaches for Realizing High Resolution, High Throughput Ion Mobility Measurements: Compressive Sensing and Ion Multiplexing**; Austen L. Davis[1]; Brian H. Clowers[1]; *[1]Washington State University, Pullman, WA*

MOF am 10:10 **Exploring Rigidity and Flexibility with Ion Mobility Mass Spectrometry: From Synthetic Knots to Disordered Proteins**; Rachelle Black[1]; Lukasz Migas[1]; Eleanor Dickinson[1]; Bruno Bellina[1]; Kamila J Pacholarz[1]; Perdita E Barran[2]; *[1]The University of Manchester, Manchester, UK; [2]The University of Manchester, Manchester, Greater Manchester*

8:30-10:30 am Monday
INSTRUMENTATION: NEW DEVELOPMENTS IN ION DETECTION
Mark Bier (Carnegie Mellon University)
Room 101-106 level 1

MOG am 08:30 **Mass and Stiffness Spectrometry based on 2D Scanning Multimode Nanomechanical Resonators for Biological Applications**; Oscar Malvar[1]; Jose Jaime Ruz[1]; Priscila Monteiro Kosaka[1]; Carmen Martínez Domínguez[1]; Eduardo Gil-Santos[1]; Dimitris Papanastasiou[2]; Monsterrat Calleja[1]; Javier Tamayo[1]; *[1]CSIC, Tres Cantos, Madrid; [2]Fasmatech Science & Technology, Athens, Greece*

MOG am 08:50 **Decreasing Uncertainty in the Mass-to-Charge Measurement in Charge Detection Mass Spectrometry with an Improved Ion Trap and Detector**; Joanna Hogan[1]; Martin Jarrold[2]; *[1]Indiana*

University, Bloomington, IN; [2]Indiana University Bloomington, Bloomington, IN

MOG am 09:10 **High Resolution Stigmatic Ion Imaging of Single Cells using a Timepix Pixel Detector**; Anne L Bruinen[1]; Rachelle Balez[2]; Nino Iakobachvili[1]; Joel Keelor[1]; Shane R. Ellis[1]; Ron MA Heeren[1]; *[1]M4I Institute - Maastricht University, Maastricht, Netherlands; [2]Illawarra Health and Medical Research Institute, School of Biological Sciences, University of Wollongong, Wollongong, Australia*

MOG am 09:30 **Development of High Intensity Biomolecular ion Beam with Quantitative and Qualitative Measurement**; Szu-Hsueh Lai[1, 2]; Jung-Lee Lin[1]; Chung-Hsuan Chen[1, 2]; *[1]Genomics Research Center Academia Sinica, Taipei; [2]National Taiwan University, Taipei, Taiwan*

MOG am 09:50 **High-Resolution Helium and Argon Isotope Analysis by Ion Counting in a Small, Multi-Turn Time-of-Flight Mass Spectrometer**; Kirk Richard Jensen[1]; Toshinobu Hondo[1, 2]; Yosuke Kawai[3]; Hirochika Sumino[4]; Michisato Toyoda[1]; *[1]Project Research Center for Fundamental Sciences, Graduate School of Science, Osaka University, Toyonaka, Japan; [2]MS-Cheminformatics, LLC, Inabe-gun, Japan; [3]Department of Earth and Space Science, Graduate School of Science, Osaka University, Toyonaka, Japan; [4]3. Department of Basic Science, Graduate School of Arts and Sciences, The University of Tokyo, Meguro-ku, Japan*

MOG am 10:10 **Novel Data Acquisition Approaches for Enhanced Ion Detection in FTMS Instruments**; Anton N. Kozhinov[1]; Konstantin O. Nagornov[1]; Yury O. Tsybin[1]; *[1]Spectroswiss Sàrl, Lausanne, Switzerland*

8:30-10:30 am Monday
SYNTHETIC POLYMERS
Chrys Wesdemiotis (University of Akron)
Room 107-110 level 1

MOH am 08:30 **Characterization of Synthetic Fibers and their Finish Layer by LAESI - MS**; Freddie van Geenen[1, 2]; Maurice Franssen[1]; Han Zuilhof[1]; Michel Nielen[1, 3]; *[1]Wageningen University, Wageningen, Netherlands; [2]TI-Coast, Amsterdam, Netherlands; [3]RIKILT Wageningen University & Research, Wageningen, Netherlands*

MOH am 08:50 **Paper Spray and Kendrick Mass Defect Analysis of Block and Random Copolymers**; Robert B. Cody[1]; Thierry Fouquet[2]; Kanae Teramoto[3]; Koji Okuda[4]; Andrew John Dane[4]; Evgeny Tishchenko[4]; *[1]JEOL USA, Inc., Peabody, MA; [2]National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan; [3]JEOL Ltd., Akishima, Japan; [4]JEOL USA Inc., Peabody, MA*

MOH am 09:10 **Improving the Resolution of the Kendrick Mass Defect Analysis of Polymer Ions with Fractional Base Units**; Thierry Fouquet[1]; Hiroaki Sato[1]; *[1]National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan*

MOH am 09:30 **Full Hydrogen/Alkali Exchange in Positive Mode Electrospray Ionization to Simplify MS/MS Reading of Information Digitally Encoded in Sequence-defined Polyurethanes**; Salomé Poyer[1]; Jean-Arthur Amalian[1]; Benoit Eric Petit[2]; Sophia Telitel[2]; Denise Karamessini[2]; Jean-François Lutz[2]; Laurence Charles[1]; *[1]Aix-Marseille University, Marseille, France; [2]Institut Charles Sadron, CNRS, Strasbourg, France*

MOH am 09:50 **Materials Compatibility Study: 3D Printer Materials**; James D Wright Jr[1]; Mary Margaret Wade[1]; Bradley Ruprecht[1]; Richard Moore[1]; Jonathan Oyler[2]; Kelly Smith[2]; *[1]US Army ECBC, APG, MD; [2]USARMY MEDCOM USAMRICD, APG, MD*

MOH am 10:10 **Thermally-Induced Reaction Mechanisms of Benzocyclobutene-Based Polymers**; Anthony Paul Gies[1]; Nathan J. Rau[1]; Liam Spencer[1]; *[1]The Dow Chemical Company, Freeport, TX*

10:30 am-2:30 pm Monday
MONDAY POSTER SESSION
Poster/Exhibit Hall
Lunch concessions are open 11:00 am-2:00 pm
Odd-number posters present 10:30 am-1:00 pm
Even-number posters present 12:00-2:30 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
MS IN CLINICAL ANALYSIS
Julie Ray (ARUP)
Hall D level 1

MOA pm 02:30 **Development and Validation of a Sensitive LC-MS/MS Method for Analysis of Milrinone in Pediatric Plasma**; Ganesh Moorthy[1]; Annie Giaccone[1]; Athena F Zuppa[1]; *[1]The Children's Hospital of Philadelphia, Philadelphia, PA*

MOA pm 02:50 **A Fast Method for the Detection of Antiepileptic Drugs in Human Urine Using Positive-Negative Polarity Switching LC-MS/MS**; Brandi R. Bridgewater[1]; Erin C. Strickland[2]; Gregory L. McIntire[2]; *[1]Ameritox, LLC, Greensboro, NC; [2]Ameritox, LLC, Greensboro, NC*

MOA pm 03:10 **Accurate Quantitation and Stability Testing of 21 Amino Acids on Dried Blood Spots by UPLC/MRM-MS**; Jun Han[1]; Rehan Higgins[1]; Juncong Yang[1]; Karen Lin[1]; Christoph H. Borchers[1, 2]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

MOA pm 03:30 **More (Sensitivity) is Always Better: Measuring Sub-clinical Levels of Thyroglobulin in Human Serum on a Micro-flow LC-MS/MS System**; Christopher M. Shuford[1]; Jay S. Johnson[2]; J. Will Thompson[3]; Patricia L. Holland[1]; James Murphy[2]; Russell P. Grant[1]; *[1]Laboratory Corporation of America, Burlington, NC; [2]Waters Corp, Milford, MA; [3]Duke University, Durham, NC*

MOA pm 03:50 **A Highly Sensitive LC-MS/MS Method for the Simultaneous Quantitation of 3α and 3β Androstane-3,17β Diol in Post-Menopausal Serum**; Yuyong Ke[1]; Alain Dury[1]; Renaud Gonthier[1]; Fernand Labrie[1]; *[1]EndoCeutics, Quebec, QC, Canada*

MOA pm 04:10 **Determination of 25-hydroxyvitamin D in Aqueous Cellular Environments by LC-MS/MS Using the Novel Chemical Derivatization Reagent MDBP**; Miriam J. Mueller[1]; Dietrich A. Volmer[1]; *[1]Saarland University, Saarbruecken, Germany*

2:30-4:30 pm Monday
ANALYTICAL CHALLENGES OF MICRODOSING AND MICROSAMPLING STUDIES
Lucinda Hittle (Merck & Co)
500 Ballroom level 1

MOB pm 02:30 **Development of Small Sample Volume Methods to Measure Drugs in Pediatric Patients: Moving Towad One-drop Blood Assays**; Liusheng Huang[1]; Janel Long-boyle[2]; Francesca Aweeka[2]; *[1]San Francisco General Hospital, UCSF, San Francisco, CA; [2]UCSF, San Francisco, CA*

MOB pm 02:50 **Dried Blood Spots in Tips Targeted Drug Screening in 9 Seconds per Sample Using Laser-Diode-Thermal-Desorption Mass Spectrometry (LDTD-MS/MS)**; Jonathan Rochon[1]; Pier-Luc Plante[2]; Serge Auger[3]; Jacques Corbeil[2]; Réal Paquin[2]; Jean Lacoursiere[3]; Pierre Picard[3]; *[1]Université Laval, Québec, QC, Canada; [2]Université Laval, Quebec, Quebec; [3]Phytronix Technologies, Québec, QC, Canada*

MOB pm 03:10 **Testing Anabolic Agents from Exhaled Breath for Doping Control Purposes Using Liquid Chromatography / High- and Low-resolution Tandem Mass Spectrometry**; Mario Thevis[1, 2]; Oliver Krug[2, 3]; Hans Geyer[2, 3]; Andreas Thomas[3]; Thomas Piper[3]; Josef Dib[3]; Andreas Lagojda[4]; Dirk Kuehne[4]; Wilhlem Schänzer[3]; *[1]German Sport University, Cologne, NRW; [2]European Monitoring Center for Emerging Doping Agents, Cologne/ Bonn, Germany; [3]German Sport University Cologne, Cologne, Germany; [4]Bayer AG, Monheim, Germany*

MOB pm 03:30 **Comprehensive Glycomic and Proteomic Profiling from Histopathological Sections of Breast Cancers: A Comparison Study of Tumor Heterogeneity**; Le Meng[1]; Nicolas Bloch[2]; Robert Pistey[2]; Joshua A. Klein[2]; Joseph Zaia[2]; *[1]Boston University School of Medicine, Boston, MA; [2]Boston University School of Medicine, Boston, MA*

MOB pm 03:50 **Mass Spectrometry Profiling of *in vitro* Tumors Using the Single-probe Device**; Xiang Tian[1]; Wei Rao[1]; Zhibo Yang[1]; *[1]University of Oklahoma, Norman, OK*

MOB pm 04:10 **Development of Chemical Isotope Labeling Nanoflow LC-MS for High-Coverage Metabolomic Profiling of 100 to 1000 Cancer Cells**; Xian Luo[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, Alberta*

2:30-4:30 pm Monday
METABOLOMICS: UNTARGETED PROFILING
Andrew Patterson (Penn State University)
Sagamore 1-3 level 2

MOC pm 02:30 **Annotation of Challenging Signals in Untargeted Metabolomics**; Nathaniel G Mahieu[1]; Gary J Patti[2]; *[1]Washington University in St. Louis, St. Louis, MO; [2]Washington University in St Louis, St. Louis, MO*

MOC pm 02:50 **Increasing Compound Identification Rates in Untargeted Metabolomics Research**; Ivana Blaženović[1]; Tobias Kind[1]; Hrvoje Torbašinović[2]; Slobodan Obrenović[2]; Sajjan S. Mehta[1]; Oliver Fiehn[1]; *[1]Metabolomics Fiehn Lab, Genome Center, University of California, Davis, California; [2]Inovatus, Zagreb, Croatia*

MOC pm 03:10 **Curated Open-access LC-Orbitrap-MS/MS Spectral Library of Endogenous Metabolites and Lipids**; Prasad Phapale; Andrew Palmer; Dominik Fay; Ivan Protsyuk; Theodore Alexandrov; *EMBL, Heidelberg, Germany*

MOC pm 03:30 **Extending a Comprehensive Reference Tandem Mass Spectral Library for More Reliable Metabolite Identification**; Xiaoyu Yang[1]; Pedatsur Neta[1]; Yuxue Liang[1]; Stephen E Stein[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

MOC pm 03:50 **Purification, Concentration and Metabolite Identification of Endogenous Urine Metabolites in Large Scale Phenotyping Studies**; Luke Whiley[1]; Elena Chekmeneva[2]; David J Berry[1]; Zoltan Takats[2]; Elaine Holmes[2]; Jeremy K Nicholson[1, 2]; Matthew Lewis[1]; *[1]MRC-NIHR National Phenome Centre, Imperial College London, London, UK; [2]Division of Computational and Systems Medicine, Department of Surgery and Cancer, Imperial College London, London, UK*

MOC pm 04:10 **Untargeted Metabolomics of 2400 American Gut Project Participants Reveals Information About Our Health, Behavior, and Microbiota**; Alan K. Jarmusch[1]; Embriette R Hyde[2]; Alexey V. Melnik[1]; Alexander Aksenov[1]; Daniel McDonald[2]; Ricardo da Silva[1]; Lindsay DeRight-Goldasich[2]; Paul Wischmeyer[3]; Rob Knight[2]; Pieter C. Dorrestein[1]; *[1]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; [2]Department of Pediatrics, University of California San Diego, La Jolla, CA; [3]Duke University School of Medicine, Durham , NC*

2:30-4:30 pm Monday
ENVIRONMENTAL: EMERGING CONTAMINANTS
Paul Chiarelli (Loyola University Chicago)
Sagamore 4 level 2

MOD pm 02:30 **Combining Non-Target and Target Screening of DBPs: Assessing Removal Strategies to Make Drinking Water Safer**; Susan Richardson[1]; Amy A. Cuthbertson[1]; Susana Y. Kimura[1]; Hannah K. Liberatore[1]; Detlef Knappe[2]; Benjamin Stanford[3]; R. Scott Summers[4]; Eric Dickenson[5]; Chad Seidel[6]; Clark Maness[2]; Riley Mulhern[4]; Amlan Ghosh[6]; Jonathan D Byer[7]; *[1]University of South Carolina, Department of Chemistry and Biochemistry, Columbia, SC; [2]North Carolina State University, Raleigh, NC; [3]Hazen and Sawyer, Raleigh, NC; [4]University of Colorado, Boulder, CO; [5]Southern Nevada Water Authority, Las Vegas, NV; [6]Corona Environmental Consulting, Boulder, CO; [7]LECO Corporation, Saint Joseph, MI*

MOD pm 02:50 **Organic Pollutants in the Clouds of the Center of France**; Olga Polyakova[1]; Viatcheslav Artaev[2]; Isabelle Canet[3]; Audrey Lallement[3]; Pierre Amato[3]; Mickael Vaitilingom[3, 4]; Anne-Marie Delort[3]; Albert T. Lebedev[1]; *[1]Moscow State University, Moscow, Russia; [2]LECO Corporation, Saint Joseph, MI; [3]Clermont Université Auvergne, CNRS, Sigma-Clermont, Institut de Chimie de Clermont-Ferrand, F-63000, Clermont-Ferrand, France; [4]Clermont Université Auvergne, CNRS, LaMP/OPGC, F-63000, Clermont-Ferrand, France*

MOD pm 03:10 **Potential Environmental Effects of Unconventional Oil and Gas Extraction: A Menu of New Mass Spectrometry Methods for Advanced Monitoring**; Doug D. Carlton[1, 2]; Zacariah L. Hildenbrand[2, 3]; Ines C. Santos[1]; Kevin A. Schug[1, 2]; *[1]The University of Texas at Arlington, Arlington, TX; [2]Affiliate of the Collaborative Laboatorires for Environmental Analysis and Remediation, The University of Texas at Arlington, Arlington, Texas; [3]Inform Environmental, LLC, Dallas, Texas*

MOD pm 03:30 **Kendrick Mass Defect Analysis in Environmental Non-target Screening: Identification of Ozonation By-products in Water Treatment**; Sylvain Merel[1]; Sascha Lege[1]; Christian Zwiener[1]; *[1]Universität Tübingen, Tübingen, Germany*

MOD pm 03:50 **Identification of Disperse Dyes in House Dust: A Novel Class of Emerging Indoor Contaminants Relevant to Human Exposure**; Lee Ferguson[1]; Heather M Stapleton[2]; *[1]Duke University, Durham, NC; [2]Duke University, Durham , NC*

MOD pm 04:10 **Determination of Nitro-Musks in Wastewater Using QuECheRS Method Combined with Electron Capture Negative Ion GC/Tandem Mass Spectrometry**; Tommy Bisbicos[1]; Grazina Pacepavicius[1]; Mehran Alaee[1]; *[1]Environment and Climate Change Canada, Burlington, ON, Canada*

2:30-4:30 pm Monday
HYDROGEN-DEUTERIUM EXCHANGE MS
Claudia Maier (Oregon State University)
Sagamore 5-7 level 2

MOE pm 02:30 **Probing the Intracellular Structure of α-synuclein by In-Cell Hydrogen/Deuterium Exchange**; Jeppe Buur Madsen[1]; Cagla Sahin[2, 3]; Daniel Otzen[2, 3]; Poul Henning Jensen[4]; Thomas J.D. Jørgensen[1]; *[1]University of Southern Denmark, Department of Biochemistry and Molecular Biology, Odense M, Denmark; [2]Aarhus University, Interdisciplinary Nanoscience Center, Aarhus C, Denmark; [3]Aarhus University, Department of Molecular Biology and Genetics, Aarhus C, Denmark; [4]Aarhus University, DANDRITE—Danish Research Institute of Translational Neuroscience & Department of Biomedicine, Aarhus C, Denmark*

MOE pm 02:50 **Analyzing Histone Dynamics Using Hydrogen-Deuterium Exchange coupled to Top-down and Middle-down Mass Spectrometry**; Kelly Karch; Mariel Coradin; Benjamin A. Garcia; *University of Pennsylvania, Philadelphia, PA*

MOE pm 03:10 **Top-down HDX Analysis of Proteins Using Ultraviolet Photodissociation**; Nicholas I. Brodie[1]; Evgeniy V. Petrotchenko[1]; Jingxi Pan[1]; Terry Zhang[2]; Romain Huguet[2]; Rosa Viner[2]; Vlad Zabrouskov[2]; Christoph H. Borchers[3, 4]; *[1]University of Victoria-Genome British Columbia Proteomics Centre, Victoria, BC, Canada; [2]Thermo Fisher Scientific, San Jose, CA; [3]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [4]Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

MOE pm 03:30 **Probing Protein Structure via Surface Induced Dissociation and Gas Phase Hydrogen-Deuterium Exchange in a Hybrid FT-ICR**; Jing Yan[1]; Arpad Somogyi[1]; Vicki H. Wysocki[1]; *[1]The Ohio State University, Columbus, OHI*

MOE pm 03:50 **Identification of Epitopes in Japanese Encephalitis Virus Envelope Protein and Characterization of Antigen Antibody Complexes by Mass Spectrometry**; Jagat Adhikari[1]; Melissa A. Edeling[2]; James Heffernan[2]; Estefania Fernandez[2]; Michael S. Diamond[2]; Daved H. Fremont[2]; Michael L. Gross[1]; *[1]Washington University, St Louis, MO; [2]Washington University School of Medicine, St Louis, MO*

MOE pm 04:10 **Hydrogen-Deuterium Exchange MS Provides Insights into Structural Dynamics of Apolipoprotein A-I and its Disease-causing Mutants on Model Discoidal High-density Lipoproteins**; Christopher Wilson[1]; Madhurima Das[2]; Xiaohu Mei[2]; Olga Gursky[2]; John R Engen[1]; *[1]Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA; [2]Department of Physiology and Biophysics, Boston University School of Medicine, Boston, MA*

2:30-4:30 pm Monday
ION MOBILITY: SMALL MOLECULES, PHARMACEUTICALS, AND DMPK
Kimberly Kew (East Carolina University)
Wabash level 1

MOF pm 02:30 **Utilising Ion-mobility Mass Spectrometry and Molecular Modelling to Screen for Synthetic Biology Targets**; Eleanor Sinclair[1]; Cunyu Yan[1]; Maria Vinaixa[1]; Perdita E Barran[1]; *[1]University of Manchester, Manchester, UK*

MOF pm 02:50 **Matrix-Assisted Ionization - Ion Mobility Spectrometry - Mass Spectrometry for the Characterization of Drugs Directly from Biological or Synthetic Environments**; Ellen D. Inutan[1, 2]; Trine G. Halvorsen[3]; Wen-Jing Zhang[1]; I-Chung Lu[1]; James Wager-Miller[4]; Srinivas B. Narayan[5]; David Crich[1]; Ken Mackie[4]; SARAH TRIMPIN[1, 2]; *[1]Department of Chemistry, Wayne State University, Detroit, MI; [2]MSTM, LLC, Newark, DE; [3]Dept. Pharmaceutical chemistry School of Pharmacy University of Oslo, Oslo, Norway; [4]Psychology and Brain Sciences, Indiana University, Bloomington, IN; [5]Detroit Medical Center University Laboratories - Core, Detroit, MI*

MOF pm 03:10 **Determination of pH-induced Oligomerization of a Lipidated Peptide by IMS-MS**; Elizabeth E Pierson[1]; Nicholas A Pierson[1]; *[1]Merck Research Laboratories, Rahway, NJ*

MOF pm 03:30 **Quantitation of Urinary Acetylcarnitine in Radiation Exposed Non-Human Primates (NHP) is Dependent upon the Calibration Curve Matrix**; Nicholas B. Vera[1, 2]; Evan Pannkuk[3]; Evagelia C. Laiakis[4]; A.J. Fornace, Jr.[4]; Stephen L. Coy[2]; Derek M. Erion[1]; Paul Vouros[2]; *[1]Pfizer, Cambridge, MA; [2]Northeastern University, Boston, MA; [3]Tumor Biology Program, Lombardi Comprehensive Cancer Center, Georgetown University, Washington, DC; [4]Georgetown University, Washington, DC*

MOF pm 03:50 **Differential Mobility – Mass Spectrometry Metabolomics Platform for Biomarker Discovery in Chronic Kidney Disease**; Stefanie Wernisch[1]; Thekkelnaycke Rajendiran[1]; Subramaniam Pennathur[1]; *[1]University of Michigan, Ann Arbor, MI*

MOF pm 04:10 **Comparison of the Selected Metal Binding Characteristics of the Methanobactin from *Methylosinus trichosporium* OB3b**; Laurence Angel[1]; Jacob W McCabe[1]; Rajpal Vangala[1]; *[1]Texas A&M University - Commerce, Commerce, TX*

2:30-4:30 pm Monday
INSTRUMENTATION: AMBIENT IONIZATION: INSTRUMENTATION & APPLICATIONS
Mari Prieto (Thermo Scientific)
Room 101-106 level 1

MOG pm 02:30 **Novel Simplified Data Mining Approach Facilitates Rapid Fingerprinting of Lignin via Ambient Ionization High-resolution Mass Spectrometry**; Elizabeth A. Crawford[1]; Stefanie Gerbig[2]; Bernhard Spengler[2]; Dietrich A. Volmer[1]; *[1]Saarland University, Saarbruecken, Germany; [2]Justus Liebig University Giessen, Giessen, Germany*

MOG pm 02:50 **Paper Spray Chemical Ionization for the Detection of Femtomole Levels of Non-polar to Less Polar Compounds**; Donghwi Kim[1]; Un Hyuk Yim[2]; Byungjoo Kim[3]; Sangwon Cha[4]; Sunghwan Kim[1]; *[1]Kyungpook National University, Daegu, South Korea; [2]Korea Institute of Ocean Science and Technology, Geoje, South Korea; [3]Korea Research Institute of Standards and Science, Daejeon, South Korea; [4]Hankuk University of Foreign Studies, Yongin, South Korea*

MOG pm 03:10 **Delayed Desorption Improves Protein Analysis by Desorption Electrospray Ionization Mass Spectrometry**; Tara L. Maser[1]; Elahe Honarvar[1]; Andre R. Venter[1]; *[1]Department of Chemistry, Western Michigan University, Kalamazoo, MI*

MOG pm 03:30 **Transmission Low Temperature Plasma Probe for *in situ* Mass Spectrometry Analysis with Paper Analytical Devices**; Yaoyao Zhao[1]; Xiaoxiao Ma[2]; Zhenwei Wei[1]; Hansen Zhao[1]; Jia Jia[1]; Sichun Zhang[1]; Zheng Ouyang[1, 2]; Xinrong Zhang[1]; *[1]Tsinghua University, Beijing, Beijing; [2]Purdue, West Lafayette, IN*

MOG pm 03:50 **Coupling of a Versatile Three-Electrode Paper-Based Electrochemical Cell to Mass Spectrometry: Electrochemical Sonic Spray Ionization Mass Spectrometry**; Yao-Min Liu[1]; Yeyoung Ha[1]; Andrew A. Gewirth[1]; *[1]University of Illinois at Urbana Champaign, Urbana, IL*

MOG pm 04:10 **Triboelectric Nanogenerators (TENGs) for Nano-Coulomb Ionization Mass Spectrometry**; Anyin Li[1]; Yunlong Zi[2]; Zhong Lin Wang[2]; Facundo M Fernandez[2]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]Georgia Institute of Technology, Atlanta, GA*

2:30-4:30 pm Monday
FUNDAMENTALS: ION-ION AND ION-NEUTRAL INTERACTIONS
Scott McLuckey (Purdue University)
Room 107-110 level 1

MOH pm 02:30 **Charge Transfer Dissociation (CTD): High Energy Radical Fragmentation of Glycans, Proteins and Peptides**; Glen Paul Jackson[1]; Pengfei Li[2]; David Ropartz[3]; Helene Rognaux[4]; *[1]West Virginia University, Morgantown, WV; [2]West Virginia University, Morgantown, WV; [3]INRA, UR1268 Biopolymers Interactions Assemblies, Nantes, France; [4]INRA, UAR1008, Nantes, France*

MOH pm 02:50 **Gas-Phase Peptide Bioconjugation with PLP and the Identification of Activation Site by Accumulative Tandem Mass Spectrometry**; Muyi HE[1]; You Jiang[2]; Sijian Ye[3]; Xiang Fang[2]; Wei Xu[1]; *[1]Beijing Institute of Technology, Beijing, Beijing; [2]National Insititute of Metrology, Beijing, China; [3]Changchun University of Science and Technology, Changchun, China*

MOH pm 03:10 **Studying Reduced Metal Complexes via Sequentially Coupled Ion/Ion-Ion/Molecule Reactions**; Mariah Parker[1]; Scott Gronert[2]; *[1]Virginia Commonwealth University, Richmond, VA; [2]Virginia Commonwealth University, Richmond, Virginia*

MOH pm 03:30 **Dual Cryogenic Ion Trap Spectrometer for Temperature-controlled Ion-molecule Reactions and Clustering**; Etienne Garand[1]; Erin M Duffy[2]; Jonathan M Voss[2]; Kaitlyn Fischer[2]; *[1]University of Wisconsin-Madison, Madison, WI; [2]University of Wisconsin-Madison, Madison, WI*

MOH pm 03:50 **Gas-phase Peptide Cross Linking for Probing the Nature of Non-covalent Bonding of a Peptide Related to Brain Damage**; Yang Liu[1]; Emilie Viglino[1]; Frantisek Turecek[1]; *[1]University of Washington, Seattle, WA*

MOH pm 04:10 **Differentiating N- Versus O-Glucuronide Metabolites via Ion/Molecule Reactions**; John Kong[1]; Zaikuan Yu[1]; Edouard Niyonsaba[1]; Ravikiran Yerabolu[1]; Xin Ma[1]; Mckay Easton[1]; Duanchen Ding[1]; Hanyu Zhu[1]; Huaming Sheng[2]; Tiffany Jarrell[2]; Zhoupeng Zhang[2]; Hilkka Kenttamaa[1]; *[1]Purdue University, West Lafayette, IN; [2]Merck & Co., Inc, Kenilworth, NJ*

4:45-5:30 pm Monday
AWARD LECTURE
Vicki Wysocki (The Ohio State University)
Hall D level 1

Award for a Distinguished Contribution in Mass Spectrometry

Catherine E. Costello
Boston University

5:45 - 7:00 PM MONDAY WORKSHOPS

There are light refreshments in common areas.

01. Improving Scientific Writing Skills
Presiding: Christopher Petucci
Room 130

"The difference between the almost right word and the right word is really a large matter - it's the difference between the lightening bug and the lightening (Mark Twain)." The ability to write grammatically correct sentences and succinct paragraphs is essential to clearly communicate ideas. This workshop will be a hands-on session for logical, clear paragraph development. Specific topics include essential grammar for scientific writing, writing grammatically correct sentences, and clearly organizing and developing your ideas in written form. At the conclusion of this session, you will have an increased knowledge of the basic writing skills to prepare manuscripts with greater clarity for theses, grant submissions, and scientific journals.

Would this workshop be of interest to the Undergraduate Research in MS and Young Mass Spectrometrists interest groups?

02. Metal Ion Coordination in Gas-Phase Bioanalysis: Reaping Practical Benefits
(Metal Ion Coordination Chemistry Interest Group)
Presiding: Cheng Lin, Eric Dodds
Room 131-132

A diverse variety of biomolecules undergo structurally and functionally significant interactions with metal ions. These interactions can be preserved in vacuo, where the resulting metalated species can exhibit characteristics quite dissimilar from those of their protonated counterparts. In the context of gas-phase bioanalysis, these differences can provide access to unique low-energy conformations, alternative dissociation pathways, or varied electronic properties. In addition, metal ion adduction can confer distinctive isotopic features and mass defect signatures. Taken together, these considerations highlight a vast yet largely untapped potential for metal ion coordination to enhance gas-phase bioanalytical strategies based on mass spectrometry, tandem mass spectrometry, and ion mobility spectrometry. This workshop will identify areas in which metal ion adduction yields advantages for biomolecular analysis spanning a wide range of application areas addressed using mass spectrometry and allied methods. Significant focus will be placed on practical guidance as discussants and participants survey new fundamental insights and emerging biological applications involving the use of metal ion charge carriers.

03. Open Source Software Packages: Using and Making your Contributions (Bioinformatics MS Interest Group)
Presiding: Samuel Payne, Meena Choi
Room 133-134

In the last 10 years, the computational mass spectrometry research community has grown dramatically as witnessed by the number of conference sessions, posters and workshops which focus on

bioinformatics and related computational topics. As the community grows, it is essential that we work to bring cooperation and collaboration to the great minds that contribute to advancing this area of science. One critical aspect of a community of interacting scientists is open source software. Although many tools for computational mass spectrometry have recently been released as open source, there remains a limited re-use of such tools. Thus, as a community, we are not yet benefiting from open source. The purpose of this workshop is to introduce several established open source packages to the community with a special emphasis on how they can use these tools in their own development of new algorithms. We will also discuss how to create proper APIs in a tool to promote re-use.

04. Clinical Diagnostics: Translating New Mass 8. Spectrometry Approaches (Clinical Chemistry Interest Group)
Presiding: Timothy Garrett
Room 135-136

The clinical lab relies on LC-MS/MS approaches, especially triple quadrupole instrumentation, for a growing number of diagnostic approaches because of the sensitivity, selectivity and specificity that mass spectrometry (coupled with chromatography) provides. In translational research the growth of new analytical techniques such as ion mobility, mass spectrometric imaging and high-resolution mass spectrometry are widely employed. Yet the translation of these techniques to clinical diagnostics is slow because of cost, ruggedness, untested performance to name a few. However, as an example, as the cost of high-resolution instruments comes closer to the purchase of a triple quad the advantages that high resolution MS have might aid clinical diagnostics. This workshop is designed to gather scientists working on clinical translational research and clinical diagnostics to discuss the challenges associated with implementation of newer MS based technologies and offer advice into the future at the adoption of new analytical MS approaches.

05. FTMS: Successes and Challenges of Achieving Routinely High Mass Accuracy (FTMS Interest Group)
Presiding: David Kilgour, Melinda McFarland
Room 137-138

This year's workshop will be a discussion focused on the experiences of the community when trying to analyse samples, to a consistently high mass accuracy, by FTMS methods. So, which factors impact mass accuracy on FT-MS instruments and when is mass uncertainty adversely affecting your results or the confidence in your results, in practice?

A lot of the discussion about mass accuracy gets passed over because one can be quite liberal with mass accuracy when working with proteomics. But, for many applications, reliably high mass accuracy is key. In this workshop we will discuss the community's experience of the mass accuracy routinely achievable in FT-MS instruments. We will discuss our success stories, times when our mass accuracy was not what was expected and what methods are used to overcome the problems.

For example do you experience non-linearity across the mass range and wonder why why resolving power is impacted by the mass range? Do you experience changes in the accuracy of the mass measurement accuracy across a chromatographic peak or in different regions of the spectrum and how could you compensate for this? How can you compensate for changes in temperature? How do the vendors try to overcome these issues? Do you have success stories where you have been able to distinguish co-eluting or co-located molecules of similar mass because of the mas accuracy you have been able to achieve?
As usual, there will be expert instrumental developers from both industry and academia to help answer your questions.

06. Exposomics Update: Success, Lessons and Future Goals (Exposomics Interest Group)
Presiding: Anthony Macherone, Skip Kingston
Room 139

The exposome compliments the genome and interrogates changes in biological response pathways resulting from exposures and integrates these with genomics and other biological information to ultimately determine the causative factors of chronic diseases. Within the exposome paradigm, exposures are defined as all bio-active chemicals circulating in the body. Examples include dietary chemicals, drugs, pollutants, metabolites, foreign DNA, reactive electrophiles adducted to human serum albumin and other sources of exposure (e.g., noise pollution, place of residence, lifestyle choices, etc.) that stimulate biochemical responses. The primary tools used in exposomic studies are mass spectrometry based in the liquid and the gas phases. These methodologies are supported by sophisticated commercial and open-source bioinformatics tools that tease out associations between the chemical information, the experimental variables and meta-data in what has come to be defined as exposome-wide association studies (EWAS).

Since 2010, at least 10 large scale exposome cohorts have been defined and funded in the USA, UK, EU, Japan and China and countless independent research initiatives have commenced - many focused on pre-natal, birth and early childhood exposures. This workshop will examine the results of exposomics studies reported in peer-reviewed literature over the past 2 - 3 years. The discussion will be focused on defining the strengths and weakness of the exposome paradigm, where innovation is needed and will attempt to define a path forward for exposome researchers.

08. Antibody-Drug Conjugate Research and Development: The Role of Multifaceted Mass Spectrometry (Pharmaceuticals Interest Group)
Presiding: Matt Schenauer, John Valliere-Douglass
Room 141-142

Due to the success of pharmaceutical interest group workshops since 2013, and broad interest in the use of MS in antibody drug-conjugate (ADC) research and development, we propose a similar workshop for 2017. After a short informal presentation (less than 15 minutes) the majority of the workshop will include an audience-driven discussion with the opportunity to ask questions to piers and a panel of experts. The short presentation will include a primer on ADCs, for those practicing mass spectrometry but unfamiliar with antibody therapeutics and their conjugates, and then provide a snapshot of current applications of MS analysis in the industry for ADC R&D. The organizers will have backup questions prepared for the panel and audience to start or prompt the discussion if needed. Potential areas of discussion may include initial Mab and drug assessments, bioanalytical assay development, and the scaling range of characterization required for ADCs as they progress through clinical development. Discussion may focus on Mass Spec method development, optimization, data analysis, and how this information is being applied within industry paradigms or changing them.

09. Forensics and Homeland Security Mass Spectrometry Research: A Critical Discussion between Academicians and Forensic Science Practitioners (Forensics & Homeland Security Interest Group)
Presiding: Adam B. Hall, Kenyon M. Evans-Nguyen
Room: 143-144

Mass spectrometry serves critical needs in forensics and homeland security for the detection of a wide variety of target compounds. The reliability of these approaches has significant effects on public safety, airport security and border protection. In order to remain vigilant and utilize modern MS-based technologies within these fields, more research is needed to address gaps in knowledge during casework and screening operations. Academicians conduct the majority of MS-based forensic science research. However, a virtual chasm exists in the translation of new technologies into practice. Implementation of new technologies is often hindered by the unusually rigorous demand of forensic techniques. Data generated by forensic practitioners must yield conclusions that can be stated with a very high degree of certainty to be useful in legal proceedings and must be generated at a lower cost than private industry. An awareness of the needs and limitations of the forensic science community can lead to more productive collaborations between researchers and practitioners. The topic, "The Research Lifecycle in Forensics and Homeland Security" will be a

critical discussion between academicians and practitioners and will work to establish effective communication through a panel discussion composed of casework focused practitioners as well as forensic scientists who are involved in casework, but also do some research. Both presiders are former practitioners who are current academicians active in research. The panel will consist of diverse perspectives to engage the audience and gain a better understanding of this critical need in the fields of forensics and homeland security.

10. Art and Cultural Heritage: Mass Spec Applications
Presiding: Mehdi Moini
Room 145

The purpose of this workshop is to discuss the application of 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 museums' specimens will be discussed in a casual, dialog format. A preliminary list of topics include: 1) Analysis of paint, coating and binders; textiles; bone and tissue; ink and paper. 2) Mechanism of aging and degradation of art and natural history objects. 3) Dating. 4) Impact of radiation on museums' specimens. 5) Fossilomics and ancient DNA. 6) Forensic archeology. 7) Species identification of proteinaceous materials used in work of art and natural history. 8) Identification of forgery.

11. Mass Spectrometry Interactive Virtual Environment (MassIVE): Management of Big Data
Presiding: Nuno Bandeira
Room 231-234

The public availability of hundreds of terabytes of mass spectrometry data have created significant challenges for the reanalysis and reutilization of proteomics and metabolomics data. This workshop will focus on ways to make MS big data accessible and easily reusable for interpretation of newly-acquired data in labs of all sizes. In particular, we i) will discuss the relative merits and pitfalls of big data MS reanalysis using advanced approaches such as proteogenomics, spectral library and blind modification searches and ii) will explore multiple ways to integrate MS big data into labs' everyday research process, including a discussion on how to make data sharing more productive and rewarding for data generating labs.

12. Ion Trap Instrumentation for Harsh Environment and Point-of-Care Applications (Ion Trap MS Interest Group)
Presiding: Zheng Ouyang, Wei Xu
Room 235-238

Ion trap has served well as an independent mass analyzer and gas-phase reactor for ion processing in hybrid instruments. In the new round of instrument development, ion trap is losing its elite status for large instruments but becoming a superior option for miniature MS systems for on-site, in-field analysis. With the strong trend of expanding MS for biomedical applications, miniature MS instruments for point-of-care analysis shall become a new focus of the instrumentation. This workshop will start with a provocative overview of the MS instrumentation development by Prof. R. Graham Cooks, followed by a series of short technical presentations and a panel discussion.

13. Photoionization: Applications, Developments, and Discussions (Photoionization MS Interest Group)
Presiding: Ralf Zimmermann, Eleanor Riches
Room 239

Photoionization is a complementary technique to other typical mass spectrometry ionization techniques, such as electrospray (ESI), electron ionization (EI), atmospheric pressure chemical ionization (APCI), etc. There are two main photoionization approaches in use today, namely Atmospheric Pressure Photoionization (APPI) and vacuum photoionization - more commonly known as single-photon ionization (SPI). APPI is commercially available and can be routinely implemented on LC-MS systems for diverse applications, whereas SPI is currently more of a research tool, although it is finding wider acceptance in several application areas - particularly those related to environmental analyses.

In this workshop, we will discuss novel applications and developments of both types of photoionization (APPI and SPI), with an opportunity for attendees to discuss their photoionization challenges and ask questions of colleagues and expert users. There will be a series of, very brief, presentations that will serve to initiate discussion around topics of key interest, including applications of both APPI and SPI, and novel developments in these fields. The aim is to help attendees understand more about the techniques and to have the chance to troubleshoot any specific issues they have encountered, thus broadening the implementation of photoionization in laboratories worldwide.

14. A Career in Mass Spec: Options and Where to start? (Young Mass Spectrometrists Interest Group)
Presiding: M. Violet Lee, Doug Phanstiel
Room 240-242

This workshop is intended to serve as a resource for young scientists interested in pursuing a career in the field of mass spectrometry. Come prepared for an interactive panel discussion on professional development with panelists from academia, government, and industry (domestic and foreign, biotech and pharma). Topics will be centered around fundamental training, internships, career options, and career planning and management.

15. Top-Down Proteomics
Presiding: Paul Thomas, Ying Ge
Room 243-245

Top Down protein mass spectrometry allows comprehensive analysis of intact, multiply modified proteoforms from complex mixtures. In this workshop, we will provide an update from the Consortium for Top Down Proteomics, discussing new community-wide pilot projects. We will also review and discuss common roadblocks to successful top down proteomics experiments from sample preparation to data acquisition to data analysis in a panel format. A limited number of 5 minute 'lightning talks' will be available for researchers to provide rapid-fire updates on recent achievements and accomplishments of note. Contact workshop chairs if you are interested in presenting.

AFTER 8:00 PM
CORPORATE HOSPITALITY SUITES
JW MARRIOTT HOTEL

From 6:45 am Tuesday
CORPORATE BREAKFAST SEMINARS
Convention Center and JW Marriott Hotel
Detailed schedule on page 15.
Pre-registration recommended, space is limited

8:30-10:30 am Tuesday
INFORMATICS: PEPTIDE AND PROTEIN IDENTIFICATION
Nuno Bandeira (UCSD)
Hall D level 1

TOA am 08:30 **PROSPEC: The PROteometools SPEctrum Compendium**; Mathias Wilhelm[1]; Daniel P Zolg[1]; Karten Schnatbaum[2]; Johannes Zerweck[2]; Tobias Knaute[2]; Bernard Delanghe[3]; Siegfried Gessulat[1]; Hans-Christian Ehrlich[4]; Maximilian Weininger[1]; Peng Yu[1]; Patroklos Samaras[1]; Judith Schlegl[5]; Karl Kramer[1]; Tobias Schmidt[1]; Holger Wenschuh[2]; Thomas Moehring[3]; Stephan Aiche[4]; Andreas F. Huhmer[6]; Ulf Reimer[2]; Bernhard Kuster[1, 7, 8]; *[1]Technical University of Munich, Freising, Germany; [2]JPT Peptide Technologies GmbH, Berlin, Germany; [3]Thermo Fisher Scientific, Bremen, Germany; [4]SAP SE, Potsdam, Germany; [5]SAP SE, Walldorf, Germany; [6]Thermo Fisher Scientific, San Jose, CA; [7]Center for Integrated Protein Science Munich, Freising, Germany; [8]Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany*

TOA am 08:50 **False Discovery Rates are Underestimated by the Target-decoy Strategy due to Unaccounted for Chemical and Biological Modifications**; Andy Kong[1]; Felipe Leprevost[1]; Dmitry M. Avtonomov[1]; Dattatreya Mellacheruvu[1]; Alexey I. Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI*

TOA am 09:10 **PTMProphet: Highly Flexible TPP Software Enables Exploration of the Known and Unknown PTM Universe with Bayesian Mixture Modeling and Beyond**; David Shteynberg[1]; Eric W. Deutsch[1]; Jimmy K Eng[2]; Andrew Keller[1]; Ulrike Kusebauch[1]; Luis Mendoza[1]; Zhi Sun[1]; Kristian Swearingen[1]; Robert L. Graham[3]; Julie A. Brazzatti[3]; Anthony Whetton[3]; Robert L. Moritz[1]; *[1]Institute for Systems Biology, Seattle, WA; [2]University of Washington Genome Sciences, Seattle, WA; [3]University of Manchester, Manchester, UK*

TOA am 09:30 **The Tale of Two Proteomes: How Data Processing Influences Cross-species Proteomic Analysis of Patient-derived Xenografts**; Arshag Mooradian[1]; Petra Erdmann-Gilmore[1]; Xuya Wang[2]; Qiang Zhang[1]; Sandeep Rajput[1]; Zhanfang Guo[1]; Jeremy Hoog[1]; Kelly V. Ruggles[2]; Sjoerd van der Post[1]; Sherri R. Davies[1]; David Fenyö[2]; Shunqiang Li[1]; Gary L. Johnson[3]; Cynthia X. Ma[1]; R. Reid Townsend[1]; Jason Held[1]; *[1]Washington University School of Medicine, St. Louis, MO; [2]New York University School of Medicine, New York, NY; [3]University of North Carolina School of Medicine, Chapel Hill, NC*

TOA am 09:50 **Covariation of Peptide Abundances Accurately Reflects Protein Concentration Difference**; Bo Zhang[1]; Mohammad Pirmoradian[1]; Roman Zubarev[1]; Lukas Käll[2]; *[1]Department of Medical Biochemistry and Biophysics, Karolinska Institutet, Solna, Sweden; [2]Royal Institute of Technology, Stockholm, Stockholm*

TOA am 10:10 **pLink2.0: Improved Search Engine for Large Scaled Cross-linked Peptides Identification**; Jia-Ming Meng[1]; Ji-Li Yin[1]; Zhen-Lin Chen[1]; Sheng-Bo Fan[1]; Yan-Jie Wu[1]; Hao Chi[1]; Chao Liu[1]; Si-Min He[1]; *[1]ICT, CAS, Beijing, China*

8:30-10:30 am Tuesday
QUANTITATIVE ANALYSIS IN DRUG DISCOVERY AND DEVELOPMENT
Petia Shipkova (Bristol Myers Squibb)
500 Ballroom level 1

TOB am 08:30 **Identification Of Contamination Of Skin Tissues Using Quantitative Mass Spectrometry Imaging**; Raphael Legouffe[1]; Stefan Linehan[2]; David Bonnel[1]; Jonathan Stauber[1]; *[1]Imabiotech, Loos, France; [2]ImaBiotech Corp, Billerica, MA*

TOB am 08:50 **Pharmacokinetic and MALDI-MSI Assessment of Orally Active Analgesic Cyclopeptides and Related Therapeutics Built on the Cyclotide Scaffold**; Aaron G Poth[1]; Brett R Hamilton[2]; Yen-Hua Huang[1]; Francis C K Chiu[3]; Thao T Le[1]; Meng-Wei Kan[1]; Michelle L Colgrave[4]; Susan A Charman[3]; Deon J Venter[2]; David J Craik[1]; *[1]Institute for Molecular Bioscience, The University of Queensland, Brisbane, Australia; [2]Mater Hospital, Brisbane, Australia; [3]Centre for Drug Candidate Optimisation, Monash Institute of Pharmaceutical Sciences, Monash University, Parkeville, Australia; [4]CSIRO, Agriculture Flagship, St Lucia, Australia*

TOB am 09:10 **Quantification of Anticancer Drug in Live Single Cancer Cells using the Single-probe Device**; Ning Pan[1]; Shawna Standke[1]; Zhibo Yang[1]; *[1]University of Oklahoma, Norman, OK*

TOB am 09:30 **Important Considerations for LC/MS-based Analysis of Tissue Distributions of Therapeutic Monoclonal Antibody**; Bo An[1]; Ming Zhang[1]; Jun Qu[1]; Yang Qu[1]; *[1]SUNY at Buffalo, Buffalo, NY*

TOB am 09:50 **Development of Quantitative Mass Spectrometry Assays for Species-matched Surrogate Antibody Fragments in Ocular Matrices**; Hilda Hernandez-Barry[1]; Robert F Kelley[2]; Devin Tesar[2]; Whitney Shatz[2]; Laetitia Comps-Agrar[2]; Joyce Chan[2]; Keyang Xu[2]; Luna Liu[2]; Yanqiu Liu[2]; Mauricio Maia[2]; Kelly Loyet[2]; *[1]Genentech, South San Francisco, CA; [2]Genentech, Inc, South San Francisco, CA*

TOB am 10:10 **Cross Platform Comparison of HRMS Instrumentation for Intact Quantitation of Biotherapeutics for PK Analysis**; Lisa A. Vasicek[1]; Alex ZHU[2]; Daniel S. Spellman[1]; Kevin Bateman[1]; *[1]Merck Reseach Labs, West Point, PA; [2]Agilent Technologies, Wilmington, DE*

8:30-10:30 am Tuesday
QUALITATIVE AND QUANTITATIVE ANALYSIS OF POST-TRANSLATIONAL MODIFICATIONS
Wei-Jun Qian (PNNL)
Sagamore 1-3 level 2

TOC am 08:30 **Determination of Absolute Phosphorylation Stoichiometry in Human Cells by Motif-targeting Quantitative Proteomics**; Chia-Feng Tsai[1, 2]; Yen-Chen Liao[1, 3]; Yi-Ting Wang[1]; Pei-Yi Lin[1]; Miao-Hsia Lin[1]; Alexey I. Nesvizhskii[4]; Yasushi Ishihama[2]; Yu-Ju Chen[1, 3]; *[1]Institute of Chemistry, Academia Sinica, Taipei, Taiwan; [2]Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; [3]Department of Chemistry, National Taiwan University, Taipei, Taiwan; [4]Department of Computational Medicine and Bioinformatics and Department of Pathology, University of Michigan Medical School, Ann Arbor, MI*

TOC am 08:50 **Targeted Dissection of Cellular Signaling Pathways by Simultaneous TOMAHAQ on Peptides and Phosphopeptides**; Brian K Erickson[1]; Devin Schweppe[1]; Joao A Paulo[1]; Alison R Erickson[1]; Jeffery Knott[2]; Steven P Gygi[1]; *[1]Harvard Medical School, Boston, MA; [2]Cell Signaling Technologies, Danvers, MA*

TOC am 09:10 **Multiplexed Kinase Pathway Monitoring using Phosphoproteomics of Effector Transcription Factors**; Alexander Federation[1]; Sandi Spencer[2]; James Bollinger[2]; John Stamatoyannopoulous[1, 2]; Michael J MacCoss[2]; *[1]Altius Institute, Seattle, WA; [2]University of Washington Genome Sciences, Seattle, WA*

TOC am 09:30 **A Dynamic Picture of the Ubiquitinome upon Proteasome Inactivation**; Jeroen AA Demmers[1]; Karen A Sap[1, 2]; Lennart van der Wal[1]; Karel Bezstarosti[1]; Dick HW Dekkers[1]; Olaf Voets[1]; Erikjan Rijkers[1]; *[1]Erasmus University Medical Center, Rotterdam; [2]Academic Medical Center Amsterdam, Amsterdam, Netherlands*

TOC am 09:50 **Site-specific Mapping of the Human SUMO Proteome Reveals Crosstalk with other Post-Translational Modifications**; Ivo Hendriks[1]; David Lyon[1]; Clifford Young[1]; Lars J Jensen[1]; Alfred CO Vertegaal[2]; Michael L Nielsen[1]; *[1]Novo Nordisk Foundation Center for Protein Research, Københavns; [2]Leiden University Medical Center, Leiden*

TOC am 10:10 **Proteome-wide Analysis of S-acylation Reveals Widespread Occurrence in Human Cells**; Bo Zhou[1]; Yiwu Yan[1]; Michael R Freeman[1]; Wei Yang[1]; *[1]Cedars-Sinai Medical Center, Los Angeles, CA*

8:30-10:30 am Tuesday
EXPOSOMICS: TARGETED, UNTARGETED AND BIOINFORMATICS METHODOLOGIES
John Bowden (NIST)
Sagamore 4 level 2

TOD am 08:30 **Integrated Mass Spectrometry-based Methods to Characterize Electronic Cigarette Exposure in Humans**; Romel P. Dator[1]; Laura Maertens[1]; Andrea Carra'[1]; Peter W. Villalta[1]; Silvia Balbo[1]; *[1]University of Minnesota, Minneapolis, MN*

TOD am 08:50 **High-coverage Metabolomic Analysis of One Microliter of Blood Using Two Isotope Labelings and High-resolution LC-MS**; Wei Han[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB, Canada*

TOD am 09:10 **Exposure Characterization of Pesticides through Untargeted Investigation of the Urinary Exposome**; Emilien L Jamin[1, 2]; Adéline Delcambre[1, 2]; Jean-François Martin[1, 2]; Nathalie Bonvallot[3]; Emmanuelle Kesse-Guyot[4]; Jean-Pierre Cravedi[1]; Laurent Debrauwer[1, 2]; *[1]Toxalim (Research Centre in Food Toxicology), Toulouse University, INRA, ENVT, INP-Purpan, UPS, Toulouse, France; [2]INRA, Platform MetaboHub-MetaToul-AXIOM, Toulouse, France; [3]EHESP – School of Public Health, Rennes – Sorbonne Paris Cité, Rennes, France; [4]Sorbonne Paris Cité Epidemiology and Statistics Research Center (CRESS), Nutritional Epidemiology Research Team (EREN), Inserm U1153, INRA U1125, Cnam, Paris13 University, Paris5 University, Paris7 University, Paris, France*

TOD am 09:30 **Gas Chromatography with Orbitrap-based High-Resolution Mass Spectrometry for Untargeted Profiling of the Human Exposome**; Douglas I. Walker[1, 2]; Yongliang Liang[1]; Annette M. Esper[1]; Greg S. Martin[1]; Gary W. Miller[2]; Dean P. Jones[1, 2]; *[1]Division of Pulmonary, Allergy and Critical Care Medicine, Department of Medicine, Emory University, Atlanta, GA; [2]HERCULES Exposome Research Center, Department of Environmental Health, Rollins School of Public Health, Emory University, Atlanta, GA*

TOD am 09:50 **Building a Library with >1000 Ion Mobility Collision Cross Sections for Ultrafast Small Molecule Analyses**; Xueyun Zheng[1]; Noor A. Aly[1]; Vanessa L. Paurus[1]; Yuxuan Zhou[1]; Daniel J. Orton[1]; Richard D. Smith[1]; Erin S Baker[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

TOD am 10:10 **Exposomics Research using Suspect Screening and Non-targeted Analysis Methods and Tools at the U.S. Environmental Protection Agency**; Elin M. Ulrich[1]; Jon R. Sobus[1]; Antony J. Williams[2]; Andrew D. McEachran[3]; Mark J. Strynar[1]; Ann M. Richard[2]; Christopher M. Grulke[2]; Seth R. Newton[1]; *[1]U.S. Environmental Protection Agency, National Exposure Research Laboratory, Research Triangle Park, NC; [2]U.S. Environmental Protection Agency, National Center for Computational Toxicology, Research Triangle Park, NC; [3]ORISE Research Participant, U.S. Environmental Protection Agency, National Center for Computational Toxicology, Research Triangle Park, NC*

8:30-10:30 am Tuesday
MACROMOLECULAR COMPLEXES
Brian Chait (Rockefeller University)
Sagamore 5-7 level 2

TOE am 08:30 **Data-driven Discovery and Validation of Human Protein Complexes via Proteome-scale Affinity-Purification Mass Spectrometry Profiling**; Edward L. Huttlin[1]; Raphael J. Bruckner[1]; Gabriela Zarraga[1]; Joe R. Cannon[1]; Lily Ting[1]; Spyros Artavanis-Tsakonas[2]; J. Wade Harper[1]; Steve Gygi[1]; *[1]Harvard Medical School, Boston, MA; [2]Biogen, Cambridge, MA*

TOE am 08:50 **Mapping the Liver Interactome**; Mark Larance[1]; Michele Tiniti[2]; Michael Ferguson[2]; Angus Lamond[2]; *[1]The University of Sydney, Camperdown, Australia; [2]University of Dundee, Dundee, UK*

TOE am 09:10 **Dynamics of the Mitochondrial Interactome**; James Bruce[1]; Juan D. Chavez[1]; Devin K. Schweppe[1]; Xuefei Zhong[1]; Chi Fung Lee[1]; Arianne Caudal[1]; Rudy Stuppard[1]; Philip A. Kramer[1]; Matthew D. Campbell[1]; David J. Marcinek[1]; Rong Tian[1]; *[1]University of Washington, Seattle, WA*

TOE am 09:30 **Endogenous Interactome of the Transcription Regulator HCF-1 Reveals Transcription Elongation as Driver of *herpesvirus* Reactivation from Latency**; Pierre M Jean Beltran[1]; Roberto Alfonso-Dunn[2]; Anne-Marie W Turner[2]; Jesse H Arbuckle[2]; Hanna G Budayeva[1]; Thomas M Kristie[2]; Ileana Cristea[1]; *[1]Princeton Universitry, Princeton, NJ; [2]NIH, Bethesda, MD*

TOE am 09:50 **High Resolution Mass Measurements Reveal Heterogeneity in Intact Ribosomal Particles**; Michiel van de Waterbeemd[1]; Kyle L Fort[1]; Dmitriy Boll[2]; Maria Reinhardt-Szyba[2]; Andrew Routh[3]; Alexander Makarov[2]; Albert J R Heck[1]; *[1]Utrecht University, Utrecht, Netherlands; [2]Thermo Fisher Scientific, Bremen, Germany; [3]University of Texas Medical Branch, Galveston, TX*

TOE am 10:10 **Charge Detection Mass Spectrometry Reveals Details of Hysteresis in Virus Capsid Disassembly**; Corinne Lutomski[1]; Nicholas Lyktey[2]; Joseph Che-Yen Wang[2]; Zhongchao Zhao[2]; Adam Zlotnick[2]; Martin Jarrold[2]; *[1]Indiana University, Bloomington , IN; [2]Indiana University, Bloomington, IN*

8:30-10:30 am Tuesday
ION MOBILITY: STRUCTURE
Carlos Larriba-Andaluz (IUPUI)
Wabash level 1

TOF am 08:30 **Direct Observation of Intermediates and Structurally Distinct Products Associated with Protein Melting Transitions by Ion Mobility**

Spectrometry-Mass Spectrometry; Tarick El-Baba[1]; Daniel W Woodall[1]; Daniel R Fuller[1]; Shannon A Raab[1]; Wen Liu[2]; Yang Liu[2]; Arthur Laganowsky[2]; David H Russell[2]; David E Clemmer[1]; *[1]Indiana University, Bloomington, IN; [2]Texas A&M University, College Station, TX*

TOF am 08:50 **Effect of Time, Temperature and Humidity on Gas Phase Protein Structure**; Juan Fernandez de la Mora[1]; Michel Attoui[2]; *[1]Yale University - Mechanical Engineering Departmen, New Haven , CT; [2]University Paris-Est Creteil, University Paris-Diderot, Paris, France*

TOF am 09:10 **Structural Dynamics of Native-like Ions: Results from Tandem Ion Mobility and Mass Spectrometry**; Samuel J. Allen[1]; Rachel M. Eaton[1]; Matthew F. Bush[1]; *[1]University of Washington, Department of Chemistry, Seattle, WA*

TOF am 09:30 **ORIGAMI: A Software Package for Data Acquisition and Analysis of Ion Mobility Collision Induced Unfolding Data from Multimeric Protein Assemblies**; Lukasz G. Migas[1]; Aidan France[1]; Bruno Bellina[1]; Kamila J. Pacholarz[1]; Perdita E. Barran[1]; *[1]University of Manchester, Manchester, UK*

TOF am 09:50 **The Reversible Coulombic-driven (un)Folding of Oligorotaxane Switches Probed by Ion Mobility Mass Spectrometry and Molecular Dynamics**; Emeline Hanozin[1]; Benoit Mignolet[2]; Denis Morsa[1]; Damien Sluysmans[3]; Anne-Sophie Duwez[3]; Fraser Stoddart[4]; Françoise Remacle[2]; Edwin De Pauw[1]; *[1]Mass Spectrometry Laboratory, Liège, Belgium; [2]Theoretical Physical Chemistry, Liège, Belgium; [3]Nanochemistry and Molecular Systems, Liège, Belgium; [4]Mechanostereochemistry Group, Evanston, IL*

TOF am 10:10 **Conformational Sampling of GHRH 1-29 Peptide Analogs using CIA-TIMS-MS**; Kevin Jeanne Dit Fouque[1]; Luis M. Salgueiro[2]; Renzhi Cai[2]; Wei Sha[2]; Andrew V. Schally[2]; Francisco A. Fernandez-Lima[1]; *[1]Department of Chemistry and Biochemistry, Florida International University, Miami, FL; [2]University of Miami School of Medicine/VA Medical Center, Department of Pathology and Department of Medicine, Divisions of Hematology/Oncology and Endocrinology and Sylvester Comprehensive Cancer Center, Miami, FL*

8:30-10:30 am Tuesday
INSTRUMENTATION: MASS ANALYZER INNOVATIONS
Ryan Danell (Danell Consulting)
Room 101-106 level 1

TOG am 08:30 **Twisted Dual-field Multipole Converging Ion Guides: Achieving High Performance in Tandem Mass Spectrometers with Reduced Size**; Haopeng Wang[1]; Laura L. Pollum[1]; Kenneth R. Newton[1]; James L. Bertsch[1]; Shane E. Tichy[1]; *[1]Agilent Technologies, Santa Clara, CA*

TOG am 08:50 **Stimulated Motion Suppression (STMS): A New Approach to Break the Resolution barrier for Ion Trap Mass Spectrometry**; Xiaoyu Zhou[1]; Xinwei Liu[1]; Wenbo Cao[1]; Ang Li[2]; Xiao Wang[3]; Zheng Ouyang[1, 3, 4]; *[1]Department of Precision Instrument, Tsinghua University, Beijing, China; [2]PurSpec Technologies Inc, Beijing, China; [3]Weldon School of Biomedical Engineering, Purdue University, West Lafayette, IN; [4]Department of Chemistry, Purdue University, West Lafayette, IN*

TOG am 09:10 **(Ultra-)High Resolution Multiple-Stage Tandem Mass Spectrometry (MS^N) in A Time-of-Flight Mass Spectrometer**; Wolfgang R Plaß[1, 2]; Wayne Lippert[1]; Timo Dickel[1, 2]; Samuel Ayet San Andres[1, 2]; Julian Bergmann[1]; Hans Geissel[1, 2]; Johannes Lang[1]; Christoph Scheidenberger[1, 2]; Wolfgang Schrader[3]; Alessandro Vetere[3]; Mikhail Yavor[4]; *[1]Justus Liebig University Giessen, Giessen, Germany; [2]GSI Helmholtz Centre for Heavy Ion Research, Darmstadt, Germany; [3]Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany; [4]Institute for Analytical Instrumentation, St. Petersburg, Russia*

TOG am 09:30 **Measuring Collisional Cross Sections of Individual Ions with Charge Detection Mass Spectrometry**; Andrew G. Elliott[1]; Conner C. Harper[1]; Haw-Wei Lin[1]; Evan R. Williams[1]; *[1]University of California, Berkeley, Berkeley, CA*

TOG am 09:50 **Phase-coherent Ion Dispersion in Non-linear Electric Fields Enables FT-ICR MS at the Cyclotron Frequency**; Konstantin O. Nagornov[1]; Edith Nicol[2]; Anton N. Kozhinov[1]; Yury O. Tsybin[1]; *[1]Spectroswiss Sàrl, Lausanne, Switzerland; [2]Ecole Polytechnique, Palaiseau, France*

TOG am 10:10 **Extension of Orbitrap Capabilities to Enable New Applications**; Alexander Makarov[1]; Erik Cousijn[1]; Jesse Canterbury[2]; Eduard Denisov[1]; Christian Thoeing[1]; Oliver Lange[1]; Arne Kreutzmann[1]; Konstantin Ayzikov[1]; Eugen Damoc[1]; Arrey Tabiwang[1]; Yue Xuan[1]; Seema Sharma[2]; Romain Huguet[2]; Graeme McAlister[2]; Mike Senko[2]; Vlad Zabrouskov[2]; Alexander Harder[1]; *[1]Thermo Fisher Scientific, Bremen, Germany; [2]ThermoFisher, San Jose, CA*

8:30-10:30 am Tuesday
FUNDAMENTALS: ION SPECTROSCOPY
Etienne Garand (University of Wisconsin)
Room 107-110 level 1

TOH am 08:30 **Water Microsolvation Switches the Binding Mode of Ni(II)Triglycine From Iminol to Charge-Solvation**; Robert C. Dunbar[1]; Jonathan K. Martens[2]; Giel Berden[2]; Jos Oomens[2, 3]; *[1]Case Western Reserve Univ, Cleveland, OH; [2]Radboud University, Nijmegen; [3]University of Amsterdam, Amsterdam, Netherlands*

TOH am 08:50 **The Molecular Structure of Electron Transfer Dissociation Product Ions Investigated using Infrared Ion Spectroscopy**; Lisanne Kempkes[1]; Jonathan Martens[1]; Giel Berden[1]; Jos Oomens[1]; *[1]FELIX Facility, Radboud University, Netherlands*

TOH am 09:10 **Analysis of Perfluorocarbons Compounds (PFCs), Potent Greenhouses Gases by Action Spectroscopy**; Suzie Douix[1]; Héloïse Dossmann[2]; Laurent Nahon[1]; Alexandre Giuliani[3]; *[1]Synchrotron Soleil, Saint Aubin, France; [2]Université Pierre et Marie Curie, Paris, France; [3]Institutal National de la Recherche Agronomique, Paris, France*

TOH am 09:30 **The Structure of the Anionic Serine Octamer**; Jongcheol Seo[1]; Stephan Warnke[1]; Kevin Pagel[1, 2]; Michael T. Bowers[3]; Gert von Helden[1]; *[1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Berlin; [2]Freie Universität Berlin, Berlin, Germany; [3]University of California Santa Barbara, Santa Barbara, CA*

TOH am 09:50 **Conformation-Specific Infrared and Ultraviolet Spectroscopy of Cold [YAPAA+H]+ and [YGPAA+H]+ Ions: A Stereochemical "Twist" on the β-Hairpin Turn**; Andrew DeBlase[1]; Christopher P Harrilal[2]; John T Lawler[2]; Nicole L Burke[2]; Scott A McLuckey[2]; Timothy S Zwier[2]; *[1]Purdue University, West Lafayette, IN; [2]Purdue University, West Lafayette, IN*

TOH am 10:10 **Combining Mass Spectrometry, Ion Mobility and Cryogenic Ion Spectroscopy for Structural Assignment of Oligosaccharides**; Chiara Masellis[1]; Neelam Khanal[2]; David E Clemmer[2]; Michael Z. Kamrath[1]; Thomas R. Rizzo[1]; *[1]EPFL, Lausanne, Switzerland; [2]Indiana University, Bloomington, IN*

10:30 am-2:30 pm Tuesday
TUESDAY POSTER SESSION
Poster/Exhibit Hall
Lunch concessions are open 11:00 am-2:00 pm
Odd-number posters present 10:30 am-1:00 pm
Even-number posters present 12:00-2:30 pm

TUESDAY AFTERNOON ORAL SESSIONS

2:30-4:30 pm Tuesday
INFORMATICS: METABOLOMICS
XiuXia Du (UNC Charlotte)
Hall D level 1

TOA pm 02:30 **Towards a Comprehensive Virtual Research Infrastructure for Large-scale Processing of Metabolomics Data and Analysing Medical Metabolic Phenome Data**; Thomas Hankemeier[1]; Michael S van Vliet[1]; Amy C Harms[1]; Alberto Pasamontes Funez[1]; Merlijn van Rijswijk[2]; Steffen Neumann[3]; Ola Spjuth[4]; Etienne Thevenot[5]; Fabien Jourdan[6]; Tim Ebbels[7]; Robert Glen[7]; Susanna-Assunta Sansone[8]; Christoph Steinbeck[9]; *[1]Leiden University, Leiden, Netherlands; [2]Netherlands Metabolomics Centre, Utrecht, Netherlands; [3]Leibniz Institute for plant Biochemistry, Halle (Saale), Germany; [4]Uppsala University, Uppsala , Sweden; [5]CEA Saclay, Gif-sur-Yvette, France; [6]INRA, Platform MetaboHub-MetaToul-AXIOM, Toulouse, France; [7]Department of Surgery and Cancer, Imperial College, London, UK; [8]Oxford e-Research Centre, Oxford, UK; [9]EMBL-EBI, Cambridge, Cambridgeshire*

TOA pm 02:50 **Hybrid Search: A Library-based Method for Identifying Metabolites Not in Tandem Mass Spectrometry Libraries**; Brian T. Cooper[1, 2]; Stephen E. Stein[2]; Xinjian Yan[2]; Yamil Simón-Manso[2]; Dmitrii V. Tchekhovskoi[2]; Yuri A. Mirokhin[2]; *[1]UNC Charlotte, Charlotte, NC; [2]NIST, Gaithersburg, MD*

TOA pm 03:10 **Development of an Expert System to Enhance Gas Chromatography-Mass Spectrometry-Based Metabolite Identification**; Feng Qiu[1]; Zhentian Lei[1]; Lloyd W. Sumner[1]; *[1]University of Missouri, Columbia, MO*

TOA pm 03:30 **Enhancing Computational Tools for Automated Ion Mobility-Mass Spectrometry-Based Small Molecule Workflows and Improved Multidimensional Analyses**; Aivett Bilbao[1]; Xueyun Zheng[1]; Bryson C. Gibbons[1]; Ed Darland[2]; Emma E. Rennie[2]; Richard D. Smith[1]; Erin S. Baker[1]; Thomas O. Metz[1]; John Fjeldsted[2]; Samuel H. Payne[1]; *[1]Earth and Biological Sciences Directorate, Pacific Northwest National Laboratory, Richland, WA; [2]Agilent Technologies, Santa Clara, CA*

TOA pm 03:50 **A Cellular Dashboard for Graphical Analysis of Metabolomics Data**; Peter Karp[1]; Suzanne Paley[1]; Paul O'Maille[1]; *[1]SRI International, Menlo Park, CA*

TOA pm 04:10 **Untargeted Metabolomics Suffers from Incomplete Data Analysis**; Richard Baran; *Baran Bioscience, LLC, Berkeley, CA*

2:30-4:30 pm Tuesday
MS IN THE REGULATORY ENVIRONMENT
Whitney Stutts (FDA)
500 Ballroom level 1

TOB pm 02:30 **Accurate Mass Fragment Library of Nootropic Compounds using DART-HRAM-MS**; Sara Kern[1]; Valerie M. Toomey[1]; Lisa M. Lorenz[1]; Jonathan J. Litzau[1]; *[1]USFDA Forensic Chemistry Center, Cincinnati, OH*

TOB pm 02:50 **High Resolution Approaches for the Identification of Environmental Metabolites**; Jeffrey Gilbert[1]; Jesse L. Balcer[1]; Yelena Adelfinskaya[1]; David G. McCaskill[1]; Shusheng Lu[1]; Kyung Myung[1]; Pete Johnson[1]; *[1]Dow AgroSciences, Indianapolis, IN*

TOB pm 03:10 **A Novel Screening Workflow using Ion-Mobility-Mass Spectrometry for the Analysis of Extractable and Leachable Components from Common Packaging Material**; Jane Cooper[1]; Oliver Burt[1]; Baiba Cabovska[2]; Chris Stumpf[2]; *[1]Waters Corp., Wilmslow, UK; [2]Waters Corp, Milford, MA*

TOB pm 03:30 **Identification and Relative Quantitation of Oxytocin Degradation Products under Accelerated Stress conditions using Liquid Chromatography-high Resolution Mass Spectrometry (LC-HRMS)**; Jinhui Zhang[1]; Ahmed Zidan[1]; Patrick J Faustino[1]; *[1]FDA, Silver Spring, MD*

TOB pm 03:50 **An Alternate Approach to the Control of Polio Vaccine and Reference Standards using Quantitative Proteomics**; Terry D. Cyr[1]; Marybeth Creskey[1]; Diane Viel[1]; Tong Wu[1]; *[1]Health Canada, Ottawa, ON, Canada*

TOB pm 04:10 **A Unifying, Informatics-Based Approach to Life Cycle Management of Impurity Data in Pharmaceutical Development**; Albert Van Wyk[1]; Dmitry Mityushev[2]; Petr Kandalov[2]; Graham A. McGibbon[1]; Andrew A. Anderson[1]; *[1]ACD/Labs, Toronto, ON, Canada; [2]ACD Ltd., Moscow, Russia*

2:30-4:30 pm Tuesday
QUANTITATIVE PROTEOMICS IN SYSTEMS BIOLOGY
Brad Ackerman (Eli Lilly & Co.)
Sagamore 1-3 level 2

TOC pm 02:30 **Quantitative Mass Spectrometry Analysis of PD-L1 Protein Expression, N-glycosylation and Expression Stoichiometry with PD-1 and PD-L2 in Human Melanoma**; Carlos Morales-Betanzos[1]; Hyoungjoo Lee[1]; Paula I. Gonzalez-Ericsson[1]; Justin M. Balko[1]; Douglas B. Johnson[1]; Lisa J. Zimmerman[1]; Daniel C. Liebler[1, 2]; *[1]Vanderbilt University, Nashville, TN; [2]Protypia, LLC, Brentwood, TN*

TOC pm 02:50 **A Method for Spatially and Temporally Resolving G Protein-coupled Receptor Protein Interaction Networks in Living Cells**; Ruth Huttenhain[1, 2]; Braden T. Lobingier[1]; Kelsie Eichel[1]; Alice Y. Ting[3]; Mark Von Zastrow[1]; Nevan J. Krogan[1, 2]; *[1]UCSF, San Francisco, CA; [2]Gladstone Institutes, San Francisco, CA; [3]Stanford University, Stanford, CA*

TOC pm 03:10 **Systems Biology and Quantitative Proteomics Approaches to Studies of Mitochondrial Dysfunction for the Discovery of Friedreich's Ataxia Biomarkers**; Ian A. Blair[1]; Qingqing Wang[1]; Lili Guo[2]; Liwei Weng[2]; Ashkan Salamtipour[1]; David R. Lynch[3, 4]; Clementina Mesaros[2]; *[1]Penn SRP Center and Center of Excellence for Environmental Toxicology, University of Pennsylvania, Philadelpha, PA; [2]Penn SRP Center and Center of Excellence*

in Environmental Toxicology, University of Pennsylvania, Philadelphia, PA; [3]Department of Neurology, Chidren's Hospital of Philadelhia, Philadelphia, PA; [4]Department of Pediatrics, University of Pennsylvania, Philadelpha, PA

TOC pm 03:30 **Relative Merits of Large-Scale Networks Generated by Quantitative Protein Expression Correlation and Affinity Purification – Mass Spectrometry**; David Nusinow[1]; John Szpyt[2]; Christopher Rose[2]; Mahmoud Ghandi[3]; Edward L Huttlin[2]; Levi A Garraway[3, 4]; Steven P Gygi[2]; *[1]Harvard Medical School, Boston, MA; [2]Harvard Medical School, Boston, MA; [3]Broad Institute of MIT and Harvard, Cambridge, MA; [4]Dana Farber Cancer Institute, Boston, MA*

TOC pm 03:50 **Defining the Cross-talk between Signaling Pathways and Chromatin Modifications Occurring during Treatment of Acute Myeloid Leukemia**; Simone Sidoli[1]; Pamela J. Sung[1]; Katarzyna Kulej[1, 2]; Martin Carroll[1]; Benjamin A. Garcia[1]; *[1]University of Pennsylvania, Philadelphia, PA; [2]The Children's Hospital of Philadelphia, Philadelphia, PA*

TOC pm 04:10 **Identification of Phosphoprotein and Phosphoprotein Networks Linked to Spine Loss in Schizophrenia**; Matthew L Macdonald[1]; Megan Garver[1]; Ying Ding[1]; Harris Bell-Temin[1]; David A Lewis[1]; Robert Sweet[1]; Nathan A Yates[1]; *[1]University of Pittsburgh, Pittsburgh, PA*

2:30-4:30 pm Tuesday
ENVIRONMENTAL: NEW INSTRUMENTATION AND APPROACHES
Kerri Pratt (University of Michigan)
Sagamore 4 level 2

TOD pm 02:30 **Untargeted Profiling of Soil Metal-metabolites by LC-ICPMS-ESIMS Reveals Plant-microbe Interactions**; Rene Boiteau[1]; Jared B Shaw[2]; Ljiljana Pasa-Tolic[2]; *[1]Pacific Northwest National Lab, Richland, WA; [2]Pacific Northwest National Lab, Richland, WA*

TOD pm 02:50 **Rapid Concomitant Analysis of Pharmaceuticals in Environmental Waters by Coated Blade Spray (CBS)-Mass Spectrometry**; Justen J Poole[1]; German A Gómez-Ríos[1]; Ezel Boyacı[1]; Nathaly Reyes Garces[1]; Janusz Pawliszyn[1]; *[1]University of Waterloo, Waterloo, ON, Canada*

TOD pm 03:10 **Detection of Volatile Disinfection By-products from Indoor Swimming Pools using a Portable GC/MS System**; Douglas Martins[1]; Leonard Rorrer[1]; Mitch Wells[1]; Philip Tackett[1]; Ernest Blatchley[2, 3]; *[1]FLIR Detection, INC, West Lafayette, IN; [2]Lyles School of Civil Engineering, West Lafayette, IN; [3]Division of Environmental and Ecological Engineering, Purdue University, West Lafayette, IN*

TOD pm 03:30 **Liquid Overflow Capture Electrospray Ionization for the On-line Analysis of Aerosol Particles**; Kenneth D. Swanson[1]; Anne L. Worth[1]; Gary L. Glish[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC*

TOD pm 03:50 **Real-time Molecular Analysis of Atmospheric Aerosols by Extractive Electrospray Ionization Time-of-Flight Mass Spectrometry (EESI-TOFMS)**; Felipe D Lopez-Hilfiker[1, 2]; Veronika Pospisilova[2]; Josef Dommen[2]; Joel R. Kimmel[1, 3]; Andre Prevot[2]; Urs Baltensperger[2]; Jay G. Slowik[2]; *[1]TOFWERK, Thun, Switzerland; [2]Paul Scherrer Institute (PSI), Villigen, Switzerland; [3]Aerodyne Research, Inc, Billerica, MA*

TOD pm 04:10 **A New On-line Single-particle Laser Mass Spectrometer for Detection of Polyaromatic Hydrocarbons and Inorganic Constituents from the Same Individual Particles**; Ralf Zimmermann[1, 2]; Johannes Passig[1, 2]; Julian Schade[1]; Matthias Fuchs[2]; Markus Oster[2]; Cornelia Jäger[3]; Martin Sklorz[1]; *[1]Joint Mass Spectrometry Centre, University of Rostock, Chair of Analytical Chemistry, Rostock, Germany; [2]Joint Mass Spectrometry Centre / Cooperation Group Comprehensive Molecular Analytics, Helmholtz Zentrum München, Neuherberg, Germany; [3]3Astrophysics and Cluster Physics Group, University Jena, Jena, Germany*

2:30-4:30 pm Tuesday
COVALENT LABELING AND CHEMICAL CROSSLINKING
Yinsheng Wang (UC Riverside)
Sagamore 5-7 level 2

TOE pm 02:30 **Protein Footprinting Probes the Protein-Membrane Interactions of Nanodisc-incorporated KRAS4b-FME**; Ben Niu[1]; Don L. Rempel[1]; Xiaoying Ye[2, 3]; Que Van[2, 3]; Andrew G. Stephen[2, 3]; Michael L. Gross[1]; *[1]Washington University, St Louis, MO; [2]Frederick National Laboratory for Cancer Research, Frederick, MD; [3]Leidos Biomedical Research, Inc., Frederick, MD*

TOE pm 02:50 **Mass Spectrometric Analysis of UV and Chemical protein-DNA Cross-links in a Chromatin Model**; Alexandra Stützer[1]; Christin Kappert[1]; Aleksandar Chernev[1]; Katharina Mucek[1]; Katharina Kramer[2]; Timo Sachsenberg[3]; Oliver Kohlbacher[3]; Wolfgang Fischle[1]; Henning Urlaub[1]; *[1]Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; [2]Max Planck Institute for Plant Breeding Research, Cologne, Germany; [3]Universität Tübingen, Tübingen, Germany*

TOE pm 03:10 **The Structure of a Complete Mediator-RNA Polymerase II Preinitiation Complex Determined by Electron Microscopy and Crosslinking Mass Spectrometry**; Michael Trnka[1]; Philip J Robinson[2]; Roger D Kornberg[2]; Alma L Burlingame[1]; *[1]UCSF, San Francisco, CA; [2]Stanford University School of Medicine, Stanford, CA*

TOE pm 03:30 **Charting the Human Nuclear Protein-protein Interaction Landscape through Cross-linking Mass Spectrometry**; Domenico Fasci[1]; Richard A. Scheltema[1]; Albert J. R. Heck[1]; *[1]Utrecht University, Utrecht*

TOE pm 03:50 **Integrative Structural Proteomics of the Native Nuclear Pore Complex**; Yi Shi[1]; Javier Fernandez-Martinez[2]; Seung Joong Kim[3]; Paula Upla[4]; Riccardo Pellarin[3]; Michael Gagnon[5]; Ilan Chemmama[3]; Junjie Wang[2]; Ilona Nudelman[2]; Wenzhu Zhang[2]; Rosemary Williams[2]; William Rice[4]; David L Stokes[4]; Daniel Zenklusen[5]; Andrej Sali[3]; Micheal P Rout[2]; Brian T Chait[2]; *[1]University of Pittsburgh School of Medicine, Pittsburgh, PA; [2]The Rockefeller University, New York, NY; [3]University of San Francisco, San Francisco, CA; [4]New York University School of Medicine, New York, NY; [5]University of Montréal, Montréal, Québec*

TOE pm 04:10 **Developing an Integrated Multiplexed Quantitative Cross-linking Mass Spectrometry Platform to Determine Composition-dependent Conformational Changes of Protein Complexes**; Craig Gutierrez[1]; Haibin Mao[2]; Clinton Yu[1]; Alexander Huszaugh[3]; Rosa Viner[4]; Eric Novitsky[3]; Scott Rychnovsky[3]; Ning Zheng[2]; Lan Huang[3]; *[1]University of California, Irvine, Irvine, CA;*

[2]Department of Pharmacology and Howard Hughes Medical Institute, University of Washington, Seattle, WA; [3]University of California, Irvine, Irvine, CA; [4]ThermoFisher, San Jose, CA

2:30-4:30 pm Tuesday
MICROORGANISMS: IDENTIFICATION AND CHARACTERIZATION
Kent Voorhees (Colorado School of Mines)
Wabash level 1

TOF pm 02:30 **Optimization of Laser-Assisted Rapid Evaporative Ionization Mass Spectrometry (REIMS) for the Automated and High-Throughput Analysis of Microorganisms and Clinical Samples**; Simon Cameron[1]; Alvaro Perdones-Montero[1]; Richard Schaffer[2]; Daniel Simon[2]; Zsolt Bodai[1]; Burak Temelkuran[1]; Frances Bolt[1]; Kate Hardiman[1]; Adam Burke[1]; Emmanuelle Bardin[1]; Tony Rickards[1, 3]; Alireza Abdolrasouli[1, 3]; Guang-Zong Yang[1]; Monica Rebec[3]; Tamas Karancsi[2]; Zoltan Takats[1]; *[1]Imperial College London, London, London; [2]Waters Research Center, Budapest; [3]Imperial College Healthcare NHS Trust, London, UK*

TOF pm 02:50 **Translational Errors in Expression of Shiga Toxin from Pathogenic *Escherichia coli* as Measured by MALDI-TOF-TOF and Orbitrap Mass Spectrometry**; Clifton K. Fagerquist[1]; William J. Zaragoza[1]; *[1]USDA/ ARS, Albany, CA*

TOF pm 03:10 **MALDI and TLC MALDI of Intact Lipids for Characterizing Bacteria, Disease, and Product Quality**; Jackson O. Lay, Jr. [1]; Rohana Liyanage[1]; Jennifer Gidden[1]; *[1]University of Arkansas, Fayetteville, AR*

TOF pm 03:30 **Detecting Antibiotic Resistance by MALDI-TOF Analysis of Bacterial Membrane Glycolipids**; William E Fondrie[1]; Lisa M Leung[2]; Dudley K Strickland[1]; Robert K Ernst[2]; David R Goodlett[3]; *[1]University of Maryland School of Medicine, Baltimore, MD; [2]University of Maryland School of Dentistry, Baltimore, MD; [3]University of Maryland School of Pharmacy, Baltimore, MD*

TOF pm 03:50 **Monitoring Alterations to Bacterial Lipidome in Antimicrobial Resistance with HILIC-IM-MS**; Kelly M. Hines[1]; Brian J. Werth[2]; Libin Xu[1]; *[1]Department of Medicinal Chemistry, University of Washington, Seattle, WA; [2]Department of Pharmacy, University of Washington, Seattle, WA*

TOF pm 04:10 **Liquid Extraction Surface Analysis Mass Spectrometry for protein Analysis Directly from Clinical Isolates of *Staphylococcus aureus* and *Pseudomonas aeruginosa***; Klaudia I Kocurek[1, 2]; Leanne Stones[1]; Josephine Bunch[2]; Robin C May[1]; Helen J Cooper[1]; *[1]University of Birmingham, Birmingham, UK; [2]National Physical Laboratory, Teddington, UK*

2:30-4:30 pm Tuesday
INSTRUMENTATION: INNOVATIONS IN FT-BASED MASS ANALYZERS
David Dearden (Brigham Young University)
Room 101-106 level 1

TOG pm 02:30 **The Next Dimension in Proteomics**; Peter B. O'Connor[1]; Maria van Agthoven[2]; Yuko P. Y. Lam[2]; *[1]University of Warwick, Coventry, West Midlands; [2]University of Warwick, Coventry, UK*

TOG pm 02:50 **Frequency-tripled Detection with Minimized Contribution from other Frequency Orders and Maximized Sensitivity**; Chad R. Weisbrod[1]; Lissa C. Anderson[1]; Steve C. Beu[1]; Greg T. Blakney[1]; Nathan K. Kaiser[1]; Alan G. Marshall[1, 2]; John P. Quinn[1]; Donald F. Smith[1]; Christopher L. Hendrickson[1, 2]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]Florida State University, Tallahassee, FL*

TOG pm 03:10 **On the Utility of Higher Harmonics in Electrospray Ionization Fourier Transform Electrostatic Linear Ion Trap Mass Spectrometry**; Eric Dziekonski[1]; Joshua T. Johnson[1]; Scott A McLuckey[1]; *[1]Purdue University, West lafayette, IN*

TOG pm 03:30 **Determination of Ion Collisional Cross Section Area in an Orbitrap Mass Analyzer**; James Sanders[1]; Dustin D Holden[1]; Jennifer S. Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

TOG pm 03:50 **Coupling of the Liquid Sampling-Atmospheric Pressure Glow Discharge with an Orbitrap: A New Paradigm for High Precision Isotope Ratio Measurements**; R. Kenneth Marcus[1]; Edward Hoegg[2]; David W. Koppenaal[3]; *[1]Clemson University, Clemson, SC; [2]Clemson University, Clemson, SC; [3]Pacific Northwest National Laboratory, Richland, WA*

TOG pm 04:10 **Initial Characterization of 3D-printed High-Resolution Low Weight and Low Power Consuming Fourier transform Mass Spectrometer Based on Cassinian Ion Trap**; Eugene (Evgeny) Nikolaev[1, 2, 3]; Gleb Vladimirov[1, 2, 3]; Yury Kostyukevich[1, 2, 3]; Oleg Kharybin[1, 2, 3]; Luis Fernando Velasquez-Garcia[4]; *[1]Skolkovo Institute of Science and Technology, Skolkovo, Russia; [2]Institute of Energy Problems of Chemical Physics Russian Academy of Sciences, Moscow, Russia; [3]Moscow Institute of Physics and Technology, Dolgoprudnyj, Russia; [4]Massachusetts Institute of Technology, Cambridge, MA*

2:30-4:30 pm Tuesday
FUNDAMENTALS: ION ACTIVATION AND DISSOCIATION
Glen Jackson (West Virginia University)
Room 107-110 level 1

TOH pm 02:30 **Who's in Charge?Dissociating"Charge-Replete" and "Charge-Deplete" Proteins**; Rachel O. Loo; Michael Nshanian; Hong Nguyen; Huilin Li; Joseph A Loo; *UCLA, Los Angeles , CA*

TOH pm 02:50 **Implementation of an Ion Carpet Array for Facile and Compact Surface-Induced Dissociation**; Joshua D. Gilbert[1]; Alyssa Q. Stiving[1]; Vicki H. Wysocki[1]; *[1]Ohio State University, Columbus, OH*

TOH pm 03:10 **Photodissociation and Radical Chemistry Shine Light on Deamidation and Protein Aging**; Dylan Riggs[1]; Sonia V. Gomez[1]; Ryan R Julian[1]; *[1]University of California, Riverside, Riverside, CA*

TOH pm 03:30 **Characterization of Antigenic Bacterial Oligosaccharides via Hybrid UVPD Activation Techniques**; Peggy E Williams[1]; W. Ryan Parker[1]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

TOH pm 03:50 **Gas-phase Ozonolysis of Ionized Cholesteryl Esters: Reaction Mechanisms, Products and Kinetics**; Sarah E Hancock[1]; Alan T Maccarone[1]; Stephen J Blanksby[2]; Todd W Mitchell[1]; *[1]University of Wollongong, Wollongong, NSW; [2]Queensland University of Technology, Brisbane, Australia*

TOH pm 04:10 **Electron Induced Dissociation/Collision Induced Dissociation of Small Molecule Drugs**; Andrea F. Lopez-Clavijo[1]; Helen J. Cooper[2]; *[1]University of Bimingham, Birmingham, UK; [2]University of Birmingham, Birmingham, UK*

4:45-5:30 pm Tuesday
AWARD LECTURE
Vicki Wysocki (The Ohio State University)
Hall D level 1

Presentation of the Research Awards

- Award sponsored by Thermo Scientific by Iain Mylchreest to Peter Nemes (George Washington University).
- Award sponsored by Wasters Corporation by Lance Nicolaysen to Abraham Badu-Tawiah (The Ohio State University).

Biemann Medal

Ryan Julian
University of California, Riverside

5:45 - 7:00 PM TUESDAY WORKSHOPS

There are light refreshments in common areas.

01. Trans-Proteomic Pipeline: New Advances and Future Developments

Presiding: Luis Mendoza, Michael Hoopmann, Eric Deutsch
Room 130

The workshop will begin with a brief overview of the open-source Trans-Proteomic Pipeline (TPP) and its newest features and capabilities. We will then focus on 5 individual topics, fostering a discussion with workshop participants on the current strengths, weaknesses, and future directions for the TPP. The workshop will enable participants to describe challenges in proteomic data analysis and help drive directions in software approaches through needs of the community. The topic leads for discussion are: cross-linking analysis, integrating de novo, spectral library, and sequence database searching approaches, proteomics informatics using cloud computing infrastructure such as Amazon Web Services, analysis of post-translational modifications with PTMProphet, and analysis of SWATH-MS data. Each topic will be introduced with a brief summary of features and ideas. Then feedback and discussion by the workshop participants will be promoted.

02. Bioinformatic Approaches for Glycomics/ Glycoproteomics

Presiding: Ron Orlando
Room 131-132

Glycosylation of proteins is one of the most common protein posttranslational modifications (PTM), and the only PTM that requires structural characterization. The diverse biological roles of glycans have created a demand for bioinformatics tools to identify individual species in the complex mixtures that often include isomeric glycans obtained from biological systems. This problem is compounded by the biosynthesis of glycoprotein glycans not being template driven like the other biopolymers (DNA, RNA, and Proteins). Bioinformatic tools are needed to better identify the roles and attributes of glycan in biological systems. In this workshop, the use of different bioinformatics tools to identify individual glycans/glycopeptides from MS data will be critically described and discussed.

03. Statistics and Bioinformatics using R

Presiding: Jeffrey Jones, Ryan Benz
Room 133-134

The objectives of this workshop will be to introduce the community to the R statistical programming language, specifically the integrated development environment R studio and a few select package libraries that facilitate data manipulation and plotting, along with presenting a few mass spectrometry relevant examples. We are proposing to structure the workshop around short 5-10 minute micro presentations introducing each subject followed by several minutes of open discussion. The overall goal of this workshop is to gauge the interests of ASMS attendees towards R statistical programming and to get a better understanding of how R can best serve the community.

04. Environmental Analysis: Modern Sampling Techniques and Data Analysis (Environmental Applications Interest Group)

Presiding: Marc Engel, Imma Ferrer Achille Cappiello
Room 135-136

When modern sampling techniques, both direct and indirect, are used to analyze complex environmental samples challenging data sets are often generated. Our workshop will focus on the analysis of complex environmental samples and the use of data analysis tools and sampling techniques to generate the highest quality data for unequivocal identification. Three speakers will present 3-5 slides followed by discussion.

05. Hepatocytes: Current and Future Use in DMPK (DMPK Interest Group)

Presiding: Philip Tiller, Mark Cancilla
Room 137-138

Hepatocytes have become an integral tool in pharmaceutical research. Hepatocytes have been routinely used to generate metabolic stability/ intrinsic clearance and metabolite profile data. These assays are conducted using hepatocytes in suspension and have been, and continue to be effective assays, even though they exhibit a cell viability period of up to only 4 hours.

As more of the new chemicals being synthesized exhibit increased metabolic stability, there is a need to extend the hepatocyte incubation period to afford meaningful data. In recent years several approaches have been developed to increase the viable incubation period, such as hepatocyte relay assays, plated and co-cultured human hepatocyte systems, and these have matured, such as HepatoPak from Ascendance (Hepregen), Hurel co-cultured primary hepatocytes, 3D hepatocyte sphereoids (Organovo) and the various hepatocyte relay assays (both suspension and plated). Additional in vitro assays have also been explored with these new tools such as toxicology, transporters and biliary excretion.

Discussion will revolve on how these new hepatocyte-based tools are impacting DMPK workflows, their pros and cons and real-life experience discussions from colleagues who have hands-on experience.

06. The NIH and NSF Review and Funding Process

Presiding: Salvatore Sechi, Charles, Edmonds, Douglas Sheeley
Room 139

Many ASMS members and conference participants are supported by the National Institutes of Health or the National Science Foundation. During this workshop the general funding and review process of grant applications/proposals will be presented. Issues like identifying the best contacts, writing an effective application/proposal, and responding to the reviewers' criticisms will be discussed. Speakers will explore these issues from the perspectives of the applicant, reviewer, and administrator, with some emphasis on new investigators and training opportunities. A "mock" NIH study section presentation will provide additional insight into the review process and opportunity for discussion with NIH and NSF staff. Substantial time will be allotted for discussion and questions. NIH and NSF staff will also be available for individual discussions with investigators during scheduled "Office Hours" in the poster exhibit hall.

07. Proteomic Workflow: Unpublished Collective Practical Knowledge from Insiders (Analytical Lab Managers Interest Group)

Presiding: Emily Chen, Allis Chien
Room 140

There is no one-size-fits-all solution to the diversity of proteomic analyses that our labs handle every day. At the same time, we have to

make sensible decisions on what workflows to use, balancing scientific goals and available resources. The wisdom gained through these experiences is crucial to daily operations and consistent high-quality results, yet typically goes unpublished. This unpublished knowledge can help all of us make better decisions when performing proteomic analyses. The 2017 ASMS Analytical Lab Managers' Workshop will be dedicated to sharing these nuggets of practical wisdom. Four segments of proteomic workflows will be covered: sample preparation, liquid chromatography, mass spectrometry, and data analysis. A panel of core lab directors will introduce each topic and initiate discussion. Come join us - contribute your wisdom and learn from others in this collaborative workshop.

08. The Need for Speed: Is your LC or Mass Spectrometer the Top Gun for Improving Throughput?
(LCMS & Related Topics Interest Group)
Presiding: Erik Soderblom, Will Thompson
Room 141-142

In your current analytical workflow, is the mass spectrometer or analytical separation holding you back from higher throughput? With the increasing performance of modern MS instrumentation, including better sensitivity and scan speeds as fast as a few milliseconds, we gain the opportunity to increase either the speed in which analytes are separated prior to MS analysis or the number of analytes that are being simultaneously measured. This workshop will discuss considerations, opportunities and challenges in utilizing the increased performance of modern mass spectrometry instrumentation with various separation strategies while still maintaining quantitative fidelity within an assay. Topics will include emerging separations and MS strategies for improving throughput, with special consideration for multiplexed assay development and the challenges this presents.

09. Tracing Uncertainty in Imaging MS: Benchmarking Reproducibility, Variability, and Performance across Experiments
(Imaging MS Interest Group)
Presiding: Raf Van de Plas, Reid Groseclose
Room 143-144

Imaging MS is rapidly developing into a powerful molecular imaging modality. During its growth the focus has naturally been on developing new capabilities and increasing performance along the spatial and spectral domains. However, as the technology matures and is applied in fields such as translational medicine, pharmaceuticals, material science, and forensics, it becomes increasingly important to develop a better understanding of the technical variability in the experimental workflow. The need to exercise more advanced control over aspects such as reproducibility, stability, and variability across experiments (e.g. through systematic performance metrics) is steadily emerging across application fields, and robust solutions will be central to the long-term development of imaging MS. Various research groups have addressed the challenge of tracking and eliminating technical variation, and proposed different approaches ranging from sample preparation to instrumental and computational methods.

In this workshop, we will discuss current approaches to benchmarking and controlling reproducibility and variability across experiments. We will also try to identify the most pressing challenges ahead. The workshop will seek insight from the academic and clinical viewpoint in terms of required levels of rigor, and will also invite input from industry and governmental institutions that employ imaging MS in their assays and studies. Ultimately, we aim to discern an overall direction and set of best practices for the field, potentially complemented by a list of major challenges.

10. JASMS - Present Status and Future
Presiding: Joe Loo
Room 145

This Workshop will discuss the "nuts and bolts" of the operation of JASMS and how manuscripts are handled – from the time a manuscript is first submitted to the time the paper is published in the print journal. The important role of the manuscript reviewers in this process will be highlighted.

11. Biotherapeutics: Hot Topics
(Biotherapeutics Interest Group)
Presiding: Charles Cheng, Ashley Ruth
Room 231-234

This workshop will be a forum to discuss hot topics in the analysis of biotherapeutics by mass spectrometry. Mass spectrometry is now used for biotherapeutic analysis from discovery and throughout product development. Discussion may include a variety of topics, ranging from protein modifications, higher order structure characterization, protein batch comparability and biosimilarity, and biotherapeutic lot release testing. Recent advancements in instrumentation and software for data analysis and reporting may also be discussed based on attendee interest and interest group survey responses.

12. HDX, Covalent Labeling & Cross Linking: State-of-the-Art and Future Directions
(HDX Covalent Labeling & Cross Linking Interest Group)
Presiding: Lan Huang, David Weis
Room 235-238

Following a short organizational meeting, the workshop will provide a forum for discussing hydrogen exchange, covalent labeling, and cross-linking approaches for protein analysis (structure, function, folding, dynamics). A panel of experts will present overviews of these three distinct approaches for MS-based characterization of higher-order protein structure. The overviews will include brief introductions to the general workflows, discussions of the strengths and weaknesses of the approaches, new developments and applications, identification of current challenges, and advice to newcomers on how to enter the fields. In addition, the panel will stimulate discussions about whether different methods can be effectively integrated for comprehensive protein analysis. There will be ample time for questions and answers including an opportunity for novices/students to contribute anonymous questions on fundamentals.

13. Polymer Mass Spectrometry: Advances
(Polymeric Materials Interest Group)
Presiding: Steve Rumbelow, Christina Mastromatteo
Room 239

This workshop will be split into three sections, namely MALDI MS (current practices and approaches to method development), poster presentations and finally an open forum on questions/issues/developments in polymer analysis.

It will commence with Kevin Owens leading discussions on best practices around running MALDI MS by describing how his team run their systems at Drexel University, covering such areas as day-to-day usage, troubleshooting, method development and other potential issues that users may encounter. Delegates will be encouraged to share their experiences with this technique during this interactive session.

This is to be followed by short forum in which any delegates (particularly students) presenting posters in the Polymers Section at this conference, will be invited to give a short synopsis (no more than 3-5 minutes each) of their posters. The aim is to give these presenters an opportunity to introduce their posters and highlight any new developments or learnings. In order to keep within reasonable time constraints, potential attendees will be canvassed prior to the meeting.

Finally, delegates will be invited to ask questions about any issues with particular applications or techniques that they are either currently working on, or are interested in investigating further. This will include any discussions on shared experiences with various instrumental techniques, through to data interpretation and processing software.

14. Metabolomics: Integration into the Emerging Arena of Multi-omic Approaches (Metabolomics Interest Group)
Presiding: John Bowden
Room 240-242

As the metabolomics field continues to mature, research continues to focus on not only improving metabolite measurement, but also more recently on how to expand application and usefulness of metabolomics data. One such approach is the adaptation of multi-omics. Multi-omics

approaches aim to integrate the results of more than one 'omic' analysis, such as combining metabolomics with genomics or proteomics, in order to improve our understanding of biology. Despite its burgeoning usage, there are several considerations that the metabolomics community must interrogate, such as the potential need for new methodology and data analysis tools that must be developed for improved interpretation of multi-omic results. The experimental design must be revisited, for example, when developing methods that perform multiple omics from a single extract/extraction. Strategies to handle multi-omic data sets need to be developed, along with new ways to perform statistical analysis data and interpretation. Since metabolomics offers the phenotype, providing the most rapid measurement of health status, we need to continue exploring the nexus by which other 'omic' approaches help enhance our understanding of metabolism and more importantly, overall organism health. This workshop will provide an opportunity to discuss these the emerging concept of multi-omics as it pertains to the metabolomics community with a few short (5 min) presentations to spur discussion.

15. Mass Spectrometry and Ion Mobility: The Role of Temperature (Fundamentals Interest Group)
Presiding: Michael Van Stipdonk, Victor Ryzhov
Room 243-245

Temperature has a significant influence of mass spectrometry and ion mobility experiments. This is true whether considering, for example, the role of effective temperature on thermochemical measurements using the kinetic method or the resolving power during separations by ion mobility. The purpose of the workshop is to explore the temperature by focusing on four (4) types of experiment: (a) use of linear free energy relationships and the kinetic method to measure gas-phase acidity and basicity, (b) threshold CID measurements to measure bond dissociation energies of reaction energy barriers, (c) temperature dependent measurements of reactions in quadrupole ion traps, and (d) variable temperature ion-mobility measurements. The format of the workshop will be discussion based, moderated by four experts in the respective areas: J. C. Poutsma for the kinetic method, Peter B. Armentrout for threshold CID, Scott Gronert for variable temperature ion trap experiments and Matt Bush for the role of temperature in ion mobility measurements. We hope the workshop will provide guidance for researchers designing experiments and interpreting the data that results from the application of mass spectrometry and ion-mobility in fundamental research.

AFTER 8:00 PM
CORPORATE HOSPITALITY SUITES
JW MARRIOTT HOTEL

WEDNESDAY MORNING ORAL SESSIONS

From 6:45 am Wednesday
CORPORATE BREAKFAST SEMINARS
Convention Center and JW Marriott Hotel
Detailed schedule on page 15.
Pre-registration recommended, space is limited

8:30-10:30 am Wednesday
INFORMATICS: DATA-INDEPENDENT ACQUISITION: INNOVATIVE METHODS AND APPLICATIONS
Arthur Moseley (Duke University)
Hall D level 1

WOA am 08:30 **Molecular Phenotyping of Alzheimer's Disease in Post-Mortem-Biospecimen Samples via Data Independent Acquisition**; Jason Michael Gilmore[1]; Gennifer Merrihew[1]; Jarrett Egertson[1]; James Bollinger[1]; Amarjeet Grewall[2]; Kathy Montine[2]; Thomas Montine[2]; Michael J MacCoss[1]; *[1]University of Washington Genome Sciences, Seattle, WA; [2]Stanford School of Medicine, Stanford, CA*

WOA am 08:50 **LibMatic: A DIA-Umpire Based Pipeline to Generate Spectral Libraries for Targeted re-Extraction in DIA**; Guo Ci Teo[1]; Dattatreya Mellacheruvu[1]; Isabell Bludau[2]; Sumithra Urs[3, 4, 5]; Kevin Conlon[6]; Felipe da Veiga Leprevost[6]; Ruedi Aebersold[2]; Venkatesha Basrur[7]; Diane Marie Simeone[8]; Alexey I. Nesvizhskii[6]; *[1]Department of Pathology, University of Michigan, Ann Arbor, Ann Arbor, MI; [2]ETH Zurich, Institute of Molecular Systems Biology, Zürich, Switzerland; [3]Department of Surgery, University of Michigan, Ann Arbor, Ann Arbor, MI; [4]Pancreatic Cancer Center, University of Michigan, Ann Arbor, MI; [5]Translational Oncology Program, University of Michigan, Ann Arbor, MI; [6]Department of Pathology, University of Michigan, Ann Arbor, MI; [7]Department of Pathology, University of Michigan, Ann Arbor, MI; [8]University of Michigan School of Medicine, Ann Arbor, MI*

WOA am 09:10 **Fighting Fire with Fire: Comprehensive DIA Spectral Libraries Improve Phosphopeptide Identification and Quantification by DIA**; Alvaro Sebastian Vaca Jacome[1]; Jarrett Egertson[2]; Brian Searle[2]; Sonia Ting[2]; Adam Officer[1]; Michael J MacCoss[2]; Steven A Carr[1]; Jacob D Jaffe[1]; *[1]Broad Institute of MIT and Harvard, Cambridge, MA; [2]University of Washington, Seattle, WA*

WOA am 09:30 **Spectral Library-free DIA (DDA-free DIA) Algorithm Applied to Data Generated on a Novel Fast Scanning Orbitrap Instrument**; Roland Bruderer[1]; Lynn Verbeke[1]; Oliver M. Bernhardt[1]; Tejas Gandhi[1]; Jan Muntel[1]; Yue Xuan[2]; Lukas Reiter[1]; *[1]Biognosys, Schlieren, Zurich; [2]Thermo Fisher Scientific, Bremen, Germany*

WOA am 09:50 **Scanning Quadrupole Data Independent Acquisition: A Novel Workflow for Targeted and Discovery Proteomics**; Ute Distler[1]; Jörg Kuharev[1]; Oliver M. Bernhardt[2]; Lukas Reiter[2]; Hannes Roest[3]; Gushinder Kaur-Atwal[4]; Sarah Lennon[4]; Jason wildgoose[5]; Keith Richardson[4]; Johannes PC Vissers[4]; Stefan Tenzer[1]; *[1]University Medical Center of the Johannes Gutenbe, Mainz, Rheinland-Pfalz; [2]Biognosys, Schlieren, Zurich; [3]Stanford University School of Medicine, Stanford, California; [4]Waters Corporation, Wilmslow, UK; [5]Waters Corp., Wilmslow, UK*

WOA am 10:10 **PCprofiler: Complex-centric Analysis of Protein Correlation Profiling Datasets**; Isabell Bludau[1]; Moritz Heusel[1]; Robin Hafen[1]; George Rosenberger[1]; Max Frank[1]; Ben Collins[1]; Matthias Gstaiger[1]; Ruedi Aebersold[1]; *[1]Institute of Molecular Systems Biology, ETH Zurich, Zurich, Switzerland*

8:30-10:30 am Wednesday
FOOD SAFETY & CHEMISTRY: NON-TARGETED SCREENING
Robert Sheridan (New York Dept of Agriculture & Markets Food Laboratory)
500 Ballroom level 1

WOB am 08:30 **Decomposition/Speciation of Seafood Products by LC-HRMS with Multivariate Statistical Analysis**; Randy Self[1]; Michael G. McLendon[1]; *[1]U.S. FDA, Bothell, WA*

WOB am 08:50 **The Advantages of Using MS/MS ALL with SWATH® Acquisition for Confident Compound Identification**; Paul C. Winkler[1]; Craig Butt[2]; April Quinn-Paquet[2]; *[1]Sciex, Framingham, MA; [2]SCIEX, Framingham, MA*

WOB am 09:10 **Orthogonal Food Analysis by Surface Plasmon Resonance Biosensing - Mass Spectrometry**; Michel W. Nielen[1]; Sweccha Joshi[2]; Dick H. Hooijerink[1]; Teris A van Beek[2]; Willem Haasnoot[1]; *[1]RIKILT Wageningen University & Research, Wageningen, Netherlands; [2]Wageningen University, Wageningen, Netherlands*

WOB am 09:30 **Drift Tube Ion Mobility (DTIM) Assisted All Ions Data-independent Acquisition (DIA) Pesticide Screening**; Xin Ma[1]; Jian zhong Li[1]; *[1]Agilent Technologies, Beijing, China*

WOB am 09:50 **Evaluation of GC-MS and Rapid Evaporative Ionization Mass Spectrometry (REIMS) Platforms for Classification of Lamb Meat Flavor**; Jessica Prenni[1]; Adam L. Heuberger[2]; Corey D. Broeckling[3]; Linxing Yao[3]; Karissa Maneotis[4]; Anthony J. Midey[5]; Bindesh Shrestha[5]; James Murphy[5]; Dale Woerner[4]; *[1]Colorado State University, Fort Collins, CO; [2]Colorado State University Department of Horticulture and Landscape Architecture, Fort Collins, CO; [3]Colorado State University's Proteomics and Metabolomics Facility, Fort Collins, CO; [4]Colorado State University Department of Animal Sciences, Fort Collins, CO; [5]Waters Corporation, Milford, MA*

WOB am 10:10 **Identification of Major Chemical Constituents in *Momordica charantia* using Liquid Chromatography-Mass Spectrometry and Its Lipase Inhibitory Activity**; Joydeb Chanda[1]; Pulok Kumar Mukherjee[2]; Sayan Biswas[2]; Suvodip Banerjee[2]; Amit Kar[2]; Faraz Rashid[3]; Dipanakar Malakar[3]; Manoj Pillai[3]; *[1]School of Natural Product Studies, Kolkata, India; [2]School of Natural Product Studies, Department of Pharmaceutical Technology, Jadavpur University, Kolkata -700 032, India, Kolkata, India; [3]Sciex, Gurgaon, Haryana, India*

8:30-10:30 am Wednesday
BIOMARKERS: QUALITATIVE ANALYSIS
Sharon Pitteri (Stanford University)
Sagamore 1-3 level 2

WOC am 08:30 **Chemically Supervised, Non-Chromatographic Accelerated Small Molecule Biomarker Discovery by Multiple Reaction Monitoring (MRM) – Profiling**; Christina Ferreira[1]; Karen E Yannell[1]; Tiago JP Sobreira[1]; R. Graham Cooks[1]; *[1]Purdue University, West Lafayette, IN*

WOC am 08:50 **A Statistical Analysis into the Role of Chemical Signaling in Giant Panda Mating**; Abbey Wilson[1]; Ashli Brown Johnson[1]; Darrell Sparks[1]; Stephan Baumann[2]; *[1]Mississippi State University, Starkville, MS; [2]Agilent Technologies, Inc., Alpharetta, GA*

WOC am 09:10 **The Proteomic and Metabolomic Characterization of Exercise-Induced Sweat**; Sean Harshman[1]; Rhonda Pitsch[2]; Brian Geier[3]; Molly Fischer[4]; Maegan O'Connor[4]; Jason Eckerle[5]; Adam Strang[3]; Jennifer Martin[3]; *[1]UES Inc, Air Force Research Laboratory, WPAFB, OH; [2]Henry M. Jackson Foundation, Frederick, MD; [3]Air Force Research Laboratory, WPAFB, OH; [4]Oak Ridge Institute of Science & Education, WPAFB, OH; [5]InfoSciTex Corporation, WPAFB, OH*

WOC am 09:30 **Is Proteomics Classification of Fertilized Cells Possible - A Case Study**; Goran Mitulovic[1]; Tanja Panić-Janković[1]; Jadranka Miletić[2]; Thomas Ebner[3]; *[1]Medical University of Vienna, KIMCL, Vienna, Austria; [2]Institute of Nuclear Sciences Vinča, Vinča, Serbia; [3]Kepler Universitätsklinikum GmbH, Linz, Austria*

WOC am 09:50 **Fluorescence-Activated Cell Sorting (FACS) Coupled to Top-down Mass Spectrometry allows Cell- and Proteoform-resolved Quantitation of Lymphocytic Lineage Biomarkers** ; Kristina Srzentic[1]; Timothy K. Toby[1]; Paul Thomas[1]; Neil L Kelleher[1]; *[1]Northwestern University, Evanston, IL*

WOC am 10:10 **Unraveling the Complexity of The Gut-Brain Axis N-glycoproteome**; Mariana Barboza[1]; Gege Xu[2]; Melanie Gareau[1]; Helen Raybould[1]; Carlito Lebrilla[2]; *[1]Department of Anatomy, Physiology & Cell Biology, School of Veterinary Medicine, Davis, CA; [2]Department of Chemistry, University of California, Davis, Davis, CA*

8:30-10:30 am Wednesday
LIPIDOMICS: LIPIDS AND PROFILING
Gavin Reid (University of Melbourne)
Sagamore 4 level 2

WOD am 08:30 **Bioactive Lipids as Clinical Biomarkers of the Inflammatory and Resolution Phases During Severe Influenza Infection** ; Veronica Anania[1]; Qingling Li[1]; Jenny Jiang[1]; Carrie M. Rosenberger[1]; Wendy Sandoval[1]; Adrienne Randolph[2]; Jacqueline M. McBride[1]; W. Rodney Mathews[1]; *[1]Genentech, Inc, South San Francisco, CA; [2]Children's Hospital Boston and Harvard Medical School, Boston, MA*

WOD am 08:50 **Lipidome Isotope Labeling of Yeast (LILY) – The Potential of 13C Reference Lipids for Quantitative Lipidomics Workflows**; Evelyn Rampler[1]; Cristina Coman[2]; Gerrit Hermann[3, 4]; Robert Ahrends[2]; David Peake[5]; Bernard Delanghe[6]; Gunda Koellensperger[7]; *[1]University Vienna, Vienna, Austria; [2]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund, Germany; [3]ISOtopic Solutions, Vienna, Austria; [4]University of Vienna, Vienna, Austria; [5]Thermo Fisher Scientific, St. Jose, Austria; [6]Thermo Fisher Scientific, Bremen, Germany; [7]University of Vienna, Vienna, Austria*

WOD am 09:10 **Harmonization of Lipidomics: Final Report of the NIST Interlaboratory Exercise on Lipidomics using Standard Reference Material 1950**; John A. Bowden[1]; Alan Heckert[2]; Candice Z. Ulmer[1]; Christina Jones[1]; Jeremy Koelmel[3]; *[1]NIST, Charleston, SC; [2]NIST, Gaithersburg, MD; [3]University of Florida, Gainesville, FL*

WOD am 09:30 **Endometrial Cancer Tissue Identification by Desorption Electrospray Ionisation (DESI) Imaging**; Olivia Raglan[1, 2]; Luisa Doria[1]; Renata F Soares[1]; James McKenzie[1]; Zoltan Takats[1]; Maria Kyrgiou[1, 2]; *[1]Imperial College London, London; [2]Imperial College Healthcare NHS Trust, London, UK*

WOD am 09:50 **Comprehensive and Quantitative Lipidomic Analysis of Human Sebum**; Elizaveta Freinkman[1]; Richard J. Robinson[1]; Kelli D. Goodman[1]; Anne M. Evans[1]; Luke A.D. Miller[1]; *[1]Metabolon, Inc., Durham, NC*

WOD am 10:10 **Dynamic Cell Surface Glycolipidome Revealed by nanoLC chip-Q-TOF Mass Spectrometry**; Maurice Wong[1]; Gege Xu[1]; Dayoung Park[1]; Mariana Barboza[1]; Carlito Lebrilla[1]; *[1]University of California, Davis, Davis, CA*

8:30-10:30 am Wednesday
GLYCOPEPTIDES AND GLYCOPROTEINS
Joe Zaia (Boston University School of Medicine)
Sagamore 5-7 level 2

WOE am 08:30 **Deglycosylation by the Acidic Glycosidase PNgase H+ Enables Analysis of N-linked Glycoproteins by Hydrogen/Deuterium Exchange Mass Spectrometry**; Jeppe B. Madsen[1]; Josef

Voglmeir[2]; Gerard Comamala[3]; Ya-Min Du[2]; Pernille F. Jensen[4]; Eva C. Østerlund[1]; Morten B. Trelle[1]; Kasper D. Rand[4]; Thomas J.D. Jørgensen[1]; *[1]Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense, Denmark; [2]Glycomics and Glycan Bioengineering Research Center, College of Food Science and Technology, Nanjing Agricultural University, Nanjing, China; [3]Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; [4]Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark*

WOE am 08:50 **Comprehensive Analysis of HIV Glycosylation by Capillary Electrophoresis Separation and Ultraviolet Photodissociation**; Jolene K Diedrich[1, 2]; John R. Yates III[1, 2]; *[1]The Scripps Research Institute, La Jolla, CA; [2]Salk Institute for Biological Studies, La Jolla, CA*

WOE am 09:10 **Thousands of Glycosites Characterized via Intact Glycopeptide Analysis using Activated Ion Electron Transfer Dissociation**; Nicholas M. Riley[1]; Alexander S. Hebert[1]; Michael S. Westphall[1]; Joshua J. Coon[1]; *[1]University of Wisconsin-Madison, Madison, WI*

WOE am 09:30 **Development of Combined Phosphoproteomic and Glycoproteomic Workflows using EThcD Fragmentation**; Matthew S. Glover[1]; Qing Yu[1]; Zhengwei Chen[1]; Lingjun Li[1]; *[1]University of Wisconsin Madison, Madison, WI*

WOE am 09:50 **A Novel Hybrid Platform Coupling Reverse Phase Glycoprotein Array with LC-MS/MS to Profile Glycoproteins for Cancer Biomarker Discovery and Validation**; Li Pan[1]; Hillary Andaluz Aguilar[1]; Linna Wang[1]; Anton Iliuk[1, 2]; Andy Tao[1, 2]; *[1]Purdue University, West Lafayette, IN; [2]Tymora Analytical Operations, West Lafayette, IN*

WOE am 10:10 **Single Amino Acid Resolution of Glycosites with Top-down UVPD of Glycoproteins**; Catherine Going[1]; Romain Huguet[2]; Daniel Lopez Ferrer[2]; Vlad Zabrouskov[2]; Andreas F. Huhmer[2]; Sharon Pitteri[1]; *[1]Stanford University School of Medicine, Palo Alto, CA; [2]ThermoFisher, San Jose, CA*

8:30-10:30 am Wednesday
IMAGING: INSTRUMENTATION & METHOD DEVELOPMENT
Ben Bowen (Lawrence Berkeley National Lab)
Wabash level 1

WOF am 08:30 **Chemical and Topographical 3D-surface Imaging of non-planar Objects on the Micrometer Scale Using AP-SMALDI MSI**; Bernhard Spengler[1]; Mario Kompauer[1]; Sven Heiles[1]; *[1]Analytical Chemistry, Giessen*

WOF am 08:50 **Quantitative Secondary Ion Mass Spectrometry Imaging of Chemically Communicating Microbial Communities**; Sage J. B. Dunham[1]; Joseph F. Ellis[1]; Nameera F. Baig[2, 3]; Nydia Morales-Soto[4, 5]; Joshua D. Shrout[4, 5]; Paul W. Bohn[2, 3]; Jonathan V. Sweedler[1]; *[1]Department of Chemistry and the Beckman Institute, University of Illinois at Urbana−Champaign, Urbana, IL; [2]Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN; [3]Department of Chemical and Biomoleculer Engineering, University of Notre Dame, Notre Dame, IN; [4]Department of Civil and Environmental Engineering and Earth Sciences, University of Notre Dame, Notre Dame, IN; [5]Department of Biological Sciences, University of Notre Dame, Notre Dame, IN*

WOF am 09:10 **Emerging Modalities for Quantitative Mass Spectrometry Imaging at Atmospheric Pressure and in Vacuum**; Akos Vertes[1]; Sylwia A. Stopka[2]; Xavier A. Holmes[2]; Pranav Balan[2]; *[1]George Washington University, Washington, DC; [2]The George Washington University, Washington, DC*

WOF am 09:30 **Analysis of Tryptic Peptides and Polar Metabolites from FFPE Tissue by MALDI and LAESI MSI**; Erin H Seeley[1]; Candice M Brown[2]; Callee M Walsh[1]; *[1]Protea Biosciences, Morgantown, WV; [2]West Virginia University School of Medicine, Morgantown, WV*

WOF am 09:50 **Imaging and *in-vivo* Tissue Analysis by Infrared Laser Assisted Rapid Evaporative Ionisation MS–towards an Integrated MS-based Tissue Identification System**; Haixing Wang[1]; Zsolt Bodai[1]; Efftychios Manoli[1]; Julia Abda[1]; Dipa Gurung[1]; Burak Temelkuran[1]; Ed St. John[1]; Daniel Leff[1]; Guang-Zhong Yang[1]; Zoltan Takats[1]; *[1]Imperial College London, London*

WOF am 10:10 **Microscope Ion Imaging of Complex Surfaces Using the Pixel Imaging Mass Spectrometry Camera**; Robert Burleigh[1]; Ang Guo[1]; Felix Allum[1]; Michael Burt[1]; Mark Brouard[1]; Steve Thompson[2]; *[1]Physical & Theoretical Chemistry Department, University of Oxford, Oxford, UK; [2]Scientific Analysis Instruments Limited, Manchester, UK*

8:30-10:30 am Wednesday
INSTRUMENTATION: MS IN EXTREME ENVIRONMENTS
Tim Short (SRI International)
Room 101-106 level 1

WOG am 08:30 **Field Deployable MS for Comprehensive Atmospheric Chemistry Studies**; Benoit Plet[1]; Fred Stroh[2]; Manjula R. Canagaratna[3]; Joel Thornton[4]; Jordan E. Krechmer[3, 5, 6]; John T Jayne[3]; Douglas R. Worsnop[3, 7]; *[1]TOFWERK, Thun, Switzerland; [2]Institute of Energy and Climate Research – Stratosphere (IEK-7), Research Centre Jülich GmbH, Jülich, Germany; [3]Center for Aerosol and Cloud Chemistry, Aerodyne Research, Billerica, MA; [4]University of Washington, Seattle, WA; [5]Cooperative Institute for Research in Environmental Sciences (CIRES), Boulder, CO; [6]Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO; [7]Department of Physics, University of Helsinki, Helsinki, Finland*

WOG am 08:50 **Development of Portable GC/MS System with Benchtop Performance for Critical DoD Applications**; Leonard Rorrer[1]; Philip Tackett[1]; Daniel Sutton[1]; Krystal Roark[1]; Brent Rardin[1]; Mitch Wells[1]; *[1]FLIR Detection, INC, West Lafayette, IN*

WOG am 09:10 **Development of AC Frequency Scanning in Quadrupole Ion Traps for Planetary Exploration**; Dalton T Snyder[1]; Christopher J Pulliam[1]; Joshua Wiley[2]; Jason Duncan[3]; Graham Cooks[1]; *[1]Purdue University, West Lafayette, IN; [2]California Institute of Technology, Pasadena, CA; [3]Acuity Brands Lighting, Inc., Crawfordsville, IN*

WOG am 09:30 **Multipole Field Effects on Cylindrical Ion Trap Performance at High Background Pressures**; Dmitriy Chernookiy[1]; J. Michael Ramsey[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC*

WOG am 09:50 **Experimental Design for Studying High Velocity Molecular Impacts in the Gas Phase**; Anupriya Anupriya[1]; Sandra Osburn[1]; Brandon Turner[1]; Daniel E. Austin[1]; *[1]Brigham Young University, Provo, UT*

WOG am 10:10 **Environmental Testing and Performance Verification of the Mars Organic Molecule Analyzer (MOMA) Mass Spectrometer Under Simulated Martian Conditions**; Ryan M.

Danell[1]; Veronica T. Pinnick[2]; Andrej Grubisic[3]; Friso H.W. van Amerom[4]; Xiang Li[5]; Desmond A. Kaplan[6]; Ricardo D. Arevalo[2]; Stephanie A. Getty[2]; William B. Brinkerhoff[2]; *[1]Danell Consulting, Inc., Winterville, NC; [2]NASA Goddard Space Flight Center, Greenbelt, MD; [3]Center for Research and Exploration in Space Science and Technology (CRESST), University of Maryland, College Park, MD; [4]Mini-Mass Consulting, Inc, Hyattsville, MD; [5]Center for Research and Exploration in Space Science and Technology (CRESST), University of Maryland, Baltimore County, MD; [6]KapScience LLC, Tewksbury, MA*

8:30-10:30 am Wednesday
FUNDAMENTALS: PHOTOIONIZATION AND PHOTODISSOCIATION
Frank Turecek (University of Washington)
Room 107-110 level 1

WOH am 08:30 **Ultraviolet Activation of Peptides Using a Tunable Photon Source**; Alexandre Giuliani [1, 2]; Francis Canon[3]; Aleksandar R. Milosavljevic[1]; Laurent Nahon[1]; *[1]Synchrotron Soleil, Gif-sur-yvette , Essonne; [2]INRA, UAR1008, Nantes, France; [3]INRA, CSGA, Dijon, France*

WOH am 08:50 **Optimization of Fixed-charge and Photo-labile Derivatives for Lipid Structure Elucidation by Photodissociation**; Venkateswara R. Narreddula[1]; Nathan R. B. Boase[1]; Berwyck L. J. Poad[1]; David L. Marshall[1]; Todd W. Mitchell[2]; Adam J. Trevitt[2]; Stephen J Blanksby[1]; *[1]Queensland University of Technology, Brisbane, Australia; [2]University of Wollongong, Wollongong, Australia*

WOH am 09:10 **Exploration of Peptide Fragmentation Utilizing 213 nm Photons for UVPD and RDD**; Lance E Talbert[1]; Ryan R Julian[1]; *[1]University of California, Riverside, Riverside, CA*

WOH am 09:30 **Disentangling Radical Rearrangement Chemistry via Labile Sites and Infrared Ion Spectroscopy**; Ning Zhao[1]; Karnamohit Ranka[1]; John Stanton[1]; Nicolas Polfer[1]; *[1]University of Florida, Department of Chemistry, Gainesville, FL*

WOH am 09:50 **Improved *de novo* Sequencing of Protonated and Charge Tagged Peptides using 157 nm VUV Photodissociation.**; Nick DeGraan-Weber[1]; James P. Reilly[1]; *[1]Indiana University, Bloomington, IN*

WOH am 10:10 **Smashing It All Up (carefully!) - Combining Surface-Induced Dissociation, Ion Mobility and UV Photodissociation as a Protein Structure Interrogation Toolbox**; Alina Theisen[1]; Bruno Bellina[1]; Bin Yan[1]; Ines Camacho[1]; Alex Jones[1]; Perdita Barran[1]; *[1]University of Manchester, Manchester, UK*

10:30 am-2:30 pm Wednesday
WEDNESDAY POSTER SESSION
Poster/Exhibit Hall
Lunch concessions are open 11:00 am-2:00 pm
Odd-number posters present 10:30 am-1:00 pm
Even-number posters present 12:00-2:30 pm

WEDNESDAY AFTERNOON ORAL SESSIONS

2:30-4:30 pm Wednesday
INFORMATICS: MULTIOMICS INTEGRATION AND APPLICATIONS
Kelly Ruggles (NYU School of Medicine)
Hall D level 1

WOA pm 02:30 **Metaproteomics For The Future: Democratizing Functional Analysis of Microbiomes via Community-based Informatics Development and Dissemination**; Pratik Jagtap[1]; Bjoern Gruening[2]; James Johnson[3]; Alessandro Tanca[4]; Bart Mesuere[5]; W Judson Hervey[6]; Carolin Kolmeder[7]; Thomas Doak[8, 9]; Thilo Muth[10]; Dave Clements[11]; Praveen Kumar[1]; Thomas McGowan[1]; Clemens Blank[2]; Bernhard Renard[10]; Josh Elias[12]; Joel Rudney[1]; Timothy Griffin[1]; *[1]University of Minnesota, Minneapolis, MN; [2]Bioinformatics Group, Department of Computer Science, University of Freiburg, Freiburg, Germany; [3]University of Minnesota, Minneapolis, MN; [4]Porto Conte Ricerche, Science and Technology Park of Sardinia,, Alghero, Italy; [5]Ghent University, Ghent, Belgium; [6]Center for Bio/Molecular Science & Engineering, Naval Research Laboratory, Washington, DC; [7]University of Helsinki, Helsinki, Finland; [8]Indiana University, Bloomington, IN; [9]National Center for Genome Analysis (NCGAS), Bloomington, IN; [10]Robert Koch Institute, Berlin, Germany; [11]Johns Hopkins University, Baltimore, MD; [12]Department of Chemical & Systems Biology, Stanford University, Stanford, CA*

WOA pm 02:50 **Personalized Profiling of Diabetes: Longitudinal Multi-omics Profiles Provide Insight into Insulin Resistance**; Hannes Roest[1]; Brian Piening[1]; Wenyu Zhou[1]; Kevin Contrepois[1]; Gucci Gu[1]; Tejaswini Mishra[1]; Blake Hanson[2]; Eddy Bautista[2]; Shana Leopold[2]; Christine Yeh[1]; Daniel Spakowicz[2]; Kimberly Kukurba[1]; Dalia Perelman[1]; Colleen Craig[1]; Denis Salins[1]; Sharon Pitteri[1]; Tracey McLaughlin[1]; George Weinstock[2]; Mike Snyder[1]; *[1]Stanford University School of Medicine, Palo Alto, CA; [2]The Jackson Laboratory for Genomic Medicine, Farmington, CT*

WOA pm 03:10 **Gene Expression and Metabolomics Integration Method Defines Cancer-Specific Molecular Signatures**; Jalal K Siddiqui[1]; Elizabeth Baskin[1]; Russell Bonneville[1]; Ewy Mathe[1]; *[1]Ohio State University, Columbus, OH*

WOA pm 03:30 **Unknown Protein Isoforms Resulting from Alternative pre-mRNA splicing Identified by the Integration of Mass Spectrometry and RASL-seq**; Laura Agosto[1, 2, 3]; Simone Sidoli[1, 3]; Michael J. Mallory[1]; Kristen W. Lynch[1, 2]; Benjamin A. Garcia[1, 2, 3]; *[1]Department of Biochemistry and Biophysics, University of Pennsylvania, Philadelphia, PA; [2]Graduate Group in Biochemistry and Molecular Biophysics, University of Pennsylvania, Philadelphia, PA; [3]Penn Epigenetics Institute, Dept. of Biochemistry and Biophysics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA*

WOA pm 03:50 **Antibody Repertoire Construction for Colorectal Cancer to Identify Tumor Affinity Antibody Peptides**; Seong Won Cha[1]; Vineet Bafna[1]; *[1]UCSD, La Jolla, CA*

WOA pm 04:10 **A New Network Module in the Perseus Software for the Analysis of Diverse Omics Data**; Jan Rudolph[1]; Juergen Cox[1]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany*

2:30-4:30 pm Wednesday
FOOD SAFETY & CHEMISTRY: FOODOMICS, ALLERGENS, BACTERIA, FOODS
Christine Parker (FDA - Food Saftey and Nutrition)
500 Ballroom level 1

WOB pm 02:30 **Multi-Allergen Detection in Thermally Processed Baked Goods with Liquid Chromatography-Tandem Mass Spectrometry: A Comparison of Methods for Allergen Quantification**; Chelsea M. Coffey[1]; Timothy R. Croley[1]; *[1]U.S. Food and Drug Administration, College Park, MD*

WOB pm 02:50 **Developing a Targeted Parallel Reaction Monitoring Method for the Detection of Milk-Derived Ingredients in Complex Matrices**; Michael Krawitzky[1]; Charles Yang[2]; Melanie Downs[1]; *[1]University of Nebraska-Lincoln, Lincoln, NE; [2]Thermo Fisher Scientific, San Jose, CA*

WOB pm 03:10 **Fingerprinting NIST Human Milk reference Material (SRM 1953) by HILIC-MS/MS for the Development of Prebiotic Oligosaccharides Mass Spectral Library**; Connie Remoroza[1]; M. Lorna A De Leoz[1]; Stephen E Stein[1]; *[1]NIST, Gaithersburg, MD*

WOB pm 03:30 **Quantification of Fructose-Asparagine, an Acrylamide Precursor, in Human Foods, Animal Foods and Mouse Ceca**; Jikang Wu[1]; Anice Sabag-Daigle[1]; Brian Ahmer[1]; Vicki H. Wysocki[1]; *[1]The Ohio State University, Columbus, OH*

WOB pm 03:50 **Selective Detection and Quantification of Cyanotoxins in Algae Dietary Supplements using Alternative HRMS Strategies**; Audrey Roy-Lachapelle[1, 2]; Morgan Solliec[3]; Maryse Bouchard[1]; Sébastien Sauvé[1]; *[1]Université de Montréal, Montréal, QC, Canada; [2]Environment and Climate Change Canada, Montreal, QC, Canada; [3]École Polytechnique de Montréal, Montréal, QC, Canada*

WOB pm 04:10 **Automated High Throughput Analysis of Food Products Using REIMS and Tecan EVO System – Goose or Duck Liver Paté?**; Julia Balog[1, 2]; Richard Schaffer[1]; Steven Pringle[2, 3]; Zoltan Takats[2]; *[1]Waters Research Center, Budapest; [2]Imperial College London, London, London; [3]Waters Corporation, Wilmslow, UK*

2:30-4:30 pm Wednesday
ANTIBODIES AND ANTIBODY DRUG CONJUGATES
Yinyin Li (Rockefeller University)
Sagamore 1-3 level 2

WOC pm 02:30 **Screening Synthetic Fabs against Ebola and Marburg Virus Antigens by Native Mass Spectrometry and Hydrogen-Deuterium Exchange Mass Spectrometry**; Liuqing Shi[1]; Parmeshwar Amatya[2]; Daisy W. Leung[2]; Gaya K. Amarasinghe[2]; Michael L. Gross[3]; *[1]Washington University in St Louis, St. Louis, MO; [2]Washington University School of Medicine, St. Louis, MO; [3]Washington University in St. Louis, St. Louis, MO*

WOC pm 02:50 **Ion Mobility-Mass Spectrometry and Gas-phase Unfolding for the Quantitative Characterization of Antibody Drug Conjugates**; Yuwei Tian[1]; Brandon T Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI*

WOC pm 03:10 **Proteomic Analysis of Serum Antibody Repertoire Dynamics Post-immunization**; Stefano Bonissone[1]; Katherine Harris[2]; Nathan Trinklein[2]; Natalie Castellana[1]; *[1]Digital Proteomics, LLC., La Jolla, CA; [2]TeneoBio, Menlo Park, CA*

WOC pm 03:30 **Complete *de novo* Sequencing of Monoclonal Antibodies by Mass Spectrometry**; Yongsheng Xiao[1]; Monika Vecchi[1]; Benbo Gao[1]; Ru Wei[1]; Dingyi Wen[1]; *[1]Biogen, Cambridge, MA*

WOC pm 03:50 **Evaluation of Peptide Mapping for Identification and Quantitation of clips in Therapeutic Proteins**; Pavel V. Bondarenko[1]; Andrew Nichols[1]; Da Ren[1]; Lan Li[1]; Jiu-Li Song[1]; Le Zhang[1]; Izydor Apostol[1]; Zhongqi Zhang[1]; *[1]Amgen, Inc., Thousand Oaks, CA*

WOC pm 04:10 **Worldwide Interlaboratory Study on Monoclonal Antibody Glycosylation: Variability and Best Values**; M. Lorna A De Leoz[1]; David L Duewer[1]; Stephen E Stein[1]; *[1]National Institute of Standards & Technology, NIST, Gaithersburg, MD*

2:30-4:30 pm Wednesday
LIPIDOMICS: NEW MS TECHNOLOGIES AND APPLICATIONS
Qibin Zhang (UNC Greensboro)
Sagamore 4 level 2

WOD pm 02:30 **Letting Ozone-induced Dissociation Out of the Box: A Modular, Platform-Independent System for Implementation in Diverse Lipidomics Workflows**; Berwyck L. J. Poad[1]; Stephen J. Blanksby[1]; David L. Marshall[1]; Reuben S. Young[1]; Todd W. Mitchell[2]; J. Larry Campbell[3]; Eva Duchoslav[3]; Martin R. Green[4]; Jayne Kirk[4]; Nick Tomczyk[4]; Shane R. Ellis[5]; Martin R. L. Paine[5]; Ron M. A. Heeren[5]; *[1]Queensland University of Technology, Brisbane, Australia; [2]University of Wollongong, Wollongong, Australia; [3]SCIEX, Concord, ON, Canada; [4]Waters Corporation, Wilmslow, UK; [5]Maastricht Multi-Modal Molecular Imaging (M4I) Institute, Maastricht University, Maastricht, Netherlands*

WOD pm 02:50 **A Complete Lipidomic Approach with Capability of Quantifying C=C Location Lipid Isomers**; Wenpeng Zhang[1]; Yu Xia[2]; Zheng Ouyang[1, 2, 3]; *[1]Weldon School of Biomedical Engineering, Purdue University, West Lafayette, IN; [2]Department of Chemistry, Purdue University, West Lafayette, IN; [3]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instruments, Tsinghua University, Beijing, China*

WOD pm 03:10 **Precise Structural Characterization of Unsaturated Lipids by 213 nm UV-Photodissociation MSn**; Gavin E Reid[1]; Reiko Kiyonami[2]; Romain Huguet[2]; Christopher Mullen[2]; Seema Sharma[2]; Jesse Canterbury[2]; Jae Schwartz[2]; Vlad Zabrouskov[2]; David Peake[2]; *[1]School of Chemistry - University of Melbourne, Parkville, Australia; [2]Thermo Fisher Scientific, San Jose, CA*

WOD pm 03:30 **Ultra-sensitive, Ultra-high Resolution Lipid and Glycolipid Isomer Analyses with a Multi-pass SLIM TWIM-MS platform and CRIMP Technology**; Roza Wojcik[1]; Ian K. Webb[1]; Liulin Deng[1]; Jennifer E. Kyle[1]; Kent J. Bloodsworth[1]; Noor A. Aly[1]; Sandilya Garimella[1]; Spencer S. Prost[1]; Randolph V Norheim[1]; Karl K. Weitz[1]; Yehia M Ibrahim[1]; Erin S Baker[1]; RIChARD D. Smith[1]; *[1]PNNL, Richland, WA*

WOD pm 03:50 **Pulling Images from the Noise: Improving Sensitivity for Low-abundant Lipids through Gas Phase Fractionation and Enrichment**; Jeffrey M Spraggins[1, 2, 3]; Raf Van de Plas[1, 2, 4]; Etienne Waelkens[5, 6]; Richard M. Caprioli[1, 2, 3, 7, 8]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Biochemistry, Vanderbilt University, Nashville, TN; [3]Department of Chemistry, Vanderbilt University, Nashville, TN; [4]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [5]Dept. of Cellular and Molecular Medicine, KU Leuven, Leuven, Belgium; [6]Sybioma,*

KU Leuven, Leuven, Belgium; [7]Department of Pharmacology, Vanderbilt University, Nashville, TN; [8]Department of Medicine, Vanderbilt University, Nashville, TN

WOD pm 04:10 **Comparison of Quadrupole and Ion Trap Collision Induced Dissociation for Structure Determination of *Francisella Nnovicida* Lipid A variants.**; Alison Scott[1]; Sung Hwan Yoon[1]; Benjamin L. Oyler[2]; Jared B Shaw[3]; Dusan Velickovic[3]; Ljiljana Pasa-Tolic[3]; Robert K. Ernst[1]; David Robinson Goodlett[4]; *[1]University of Maryland School of Dentistry, Baltimore, MD; [2]University of Maryland School of Medicine, Baltimore, MD; [3]Pacific Northwest National Laboratory, Richland, WA; [4]University of Maryland School of Pharmacy, Baltimore, MD*

2:30-4:30 pm Wednesday
BIOMARKERS: QUANTITATIVE ANALYSIS
John Koomen (Moffitt Cancer Center)
Sagamore 5-7 level 2

WOE pm 02:30 **Development and Validation of Total and Isoform-specific Assays for Quantification of Periostin in Human Serum Using Immunocapture-LC-MS/MS**; Dean E McNulty[1]; Dana Knecht[1]; Jonathan Kehler[1]; Christopher A Evans[1]; Matthew Szapacs[1]; *[1]GSK, King of Prussia, PA*

WOE pm 02:50 **Systematic Evaluation of SRM-, PRM- and DIA-Based Targeted Quantification**; Ehwang Song[1]; Tujin Shi[2]; Hui Wang[2]; Anil K. Shukla[2]; Thomas L. Fillmore[2]; Yuqian Gao[2]; Ronald J. Moore[2]; Matthew J. Gaffrey[2]; Athena A. schepmoes[2]; Karin D. Rodland[2]; Richard D. Smith[2]; Wei-Jun Qian[2]; Tao Liu[2]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Pacific Northwest National Laboratory, Richland, WA*

WOE pm 03:10 **Detection of Ovarian Cancer Recurrence Using a Novel Integrated Proteomics Approach**; Ankit Sinha[1]; Ali Hussain[1]; Kwan Tang[2]; Vladimir Ignatchenko[2]; Alexandr Ignatchenko[2]; Blaise Clarke[2]; Marcus Bernardini[2]; Benjamin Neel[3]; Laurie Ailles[2]; Thomas Kislinger[2]; *[1]University of Toronto, Toronto, ON, Canada; [2]Princess Margaret Cancer Centre, Toronto, ON, Canada; [3]Perlmutter Cancer Center, NYU Langone Medical Center, New York, NY*

WOE pm 03:30 **Development of Protein Biomarkers for Radiation Injury Using Quantitative Proteomics and Mass Spectrometry**; Kate Liu[1]; Elizabeth Singer[1]; Whitaker Cohn[1]; William McBride[1]; Julian Whitelegge[1]; Joseph A Loo[1]; *[1]UCLA, Los Angeles, CA*

WOE pm 03:50 **Robust and Multiplexed Immuno-MRM Workflow for Relative Quantitation of Tumor Suppressors and Phosphopeptide Biomarkers of DNA Damage Response (DDR) Pathway**; Si Mou[1]; Lei Xiong[1]; Jeffery R. Whiteaker[2]; Lei Zhao[2]; Yihan Li[1]; Amanda G. Paulovich[2]; Hua-Fen Liu[1]; Christie Hunter[1]; *[1]SCIEX, Redwood City, CA; [2]Fred Hutchinson Cancer Research Center, Seattle, WA*

WOE pm 04:10 **Translational Top-down Proteomics as a Path Forward to Improved Diagnostics in Human Solid Organ Transplant Rejection**; Tim Toby[1]; Paul Thomas[2]; Josh Levitsky[3]; John Friedewald[3]; Michael Abecassis[3]; Neil L Kelleher[2]; *[1]Northwestern University-Kelleher Research Group, Evanston, IL; [2]Northwestern University, Chicago, IL; [3]Northwestern University Feinberg School of Medicine, Chicago, IL*

2:30-4:30 pm Wednesday
IMAGING: COMPUTATIONAL METHODS AND ANALYSIS
Erin Seeley (Protea Biosciences)
Wabash level 1

WOF pm 02:30 **MSIpad: An Effective Tool for Mass Spectrometry Metabolic Imaging, as Demonstrated by Extraction of Hormone Abnormalities in Diabetic Mouse Pancreas**; Xian Mao[1]; Tine Hectors[2]; Gerard Griffioen[2]; Bart De Moor[1]; Etienne Waelkens[3]; *[1]KU Leuven, ESAT-STADIUS / imec, Leuven, Belgium; [2]reMYND, Bio-Incubator, Leuven, Belgium; [3]KU Leuven, Dept. Cellular and Molecular Medicine, Leuven, Belgium*

WOF pm 02:50 **Software Development for Automated Statistical Classification of Clinical Samples using Ambient Mass Spectrometry**; Jonathan H Young[1]; John Lin[1]; Rob Tibshirani[2]; Livia S Eberlin[1]; *[1]Department of Chemistry, The University of Texas at Austin, Austin, TX; [2]Departments of Biomedical Data Sciences and Statistics, Stanford, CA*

WOF pm 03:10 **Data Dependent Imaging Mass Spectrometry of Serial Tissue Sections Guided by Non-linear Registration of Autofluorescence Images**; Nathan Heath Patterson[1, 2]; Nico Verbeeck[3]; Raf Van de Plas[1, 3]; Jeffrey Spraggins[1, 4]; Richard M. Caprioli[1, 4, 5, 6, 7]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Biochemistry, Vanderbilt University, Nashville, TN; [3]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [4]Department of Biochemistry, Vanderbilt University, Nasvhille, TN; [5]Department of Chemistry, Vanderbilt University, Nashville, TN; [6]Department of Pharmacology, Vanderbilt University, Nashville, TN; [7]Department of Medicine, Vanderbilt University, Nashville, TN*

WOF pm 03:30 **Automated Approach for Comprehensive Interpretation of Correlated ToF-SIMS and AFM Nanomechanical Data Based on Data Analytics**; Anton V. Ievlev[1]; Aleeza Leder Macek[1]; Ramakrishnan Kannan[1]; Stephen Jesse[1]; Mitchel J. Doktycz[1]; Scott Retterer[1]; Sergei V. Kalinin[1]; Olga S. Ovchinnikova[1]; *[1]Oak Ridge National Laboratory, Oak Ridge , TN*

WOF pm 03:50 **Optimized Processing Workflow for Improved Information Recovery from Large-scale MSI Data**; Kirill Veselkov[1]; Jonathan Sleeman[2]; Emmanuelle Claude[3]; Ivan Laponogov[1]; Mark Towers[3]; Robert Tonge[3]; Jeremy K Nicholson[1]; Zoltan Takats[1]; James Langridge[3]; *[1]Imperial College London, London, UK; [2]Center for Biomedicine and Medical Technology, Mannheim, Germany; [3]Waters Corporation, Wilmslow, UK*

WOF pm 04:10 **Big Community Data Analytics for Metabolite Imaging Mass Spectrometry**; Vitaly Kovalev[1]; Artem Tarasov[1]; Andrew Palmer[1]; Katja Ovchinnikova[1]; Dominik Fay[1]; Theodore Alexandrov[1]; *[1]EMBL, Heidelberg, Germany.* The full list of data contrbutors to METASPACE is online.

2:30-4:30 pm Wednesday
INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION AND SAMPLING
Michael MacCoss (University of Washington)
Room 101-106 level 1

WOG pm 02:30 **Mechanistic Insights and Practical Utility of Highly-Charged Protein Ions on Vacuum Source Mass Spectrometers**; Sarah Trimpin[1]; Wen-Jing Zhang[1]; I-Chung Lu[1]; Efstathios Elia[1]; Tarick J. El-Baba[1]; Corinne A. Lutomski[1]; Joshua L. Fischer[1]; Ellen D. Inutan[1, 2]; Casey D. Foley[1]; Steffen M. Weidner[3]; *[1]Department of Chemistry, Wayne State*

University, Detroit, MI; [2]MSTM, LLC, Newark, DE; [3]BAM-Federal Institute for Materials Research and Testing, Berlin, Germany

WOG pm 02:50 **Supercharging of Analytes via a Novel Modified Ion Source**; Christopher Andrew Wootton[1]; Haytham E. M. Hussein[1]; Cookson K. C. Chui[1]; Mark P Barrow[1]; Peter B. O'Connor[1]; *[1]University of Warwick, Coventry, UK*

WOG pm 03:10 **Quantitative Extraction and Ambient Analysis at a Subcellular Level**; Julia Laskin[1]; Ruichuan Yin[1]; venkateshkumar Prabhakaran[1]; Patrick El Khoury[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

WOG pm 03:30 **Analytic Directed Screening System for the Rapid Screening of Synthetic Pathways**; Michael Wleklinski[1]; Bradley P. Loren[1]; Andy Koswara[1]; Caitlin E. Falcone[1]; Zinia Jaman[1]; Kiran Iyer[1]; H. Samuel Ewan[1]; Christina R. Ferreira[1]; Yanyang Hu[1]; Kathryn Yammine[1]; Adam Hollerbach[1]; Tiago JP Sobreira[1]; Larisa Avramova[1]; David H. Thompson[1]; Zoltan K. Nagy[1]; R. Graham Cooks[1]; *[1]Purdue University, West lafayette, IN*

WOG pm 03:50 **Microsampling for Proteomic Characterization of Increasingly Smaller Cells in the Vertebrate (Frog) Embryo**; Camille Lombard-Banek[1]; Aparna B. Baxi[2]; Sally A Moody[1]; Peter Nemes[2]; *[1]George Washington University, Washington, DC; [2]George Washington University, Washington , DC*

WOG pm 04:10 **An Open Port Sampling Interface as a Noncontact Injection System for Coupling Liquid droplet sample Dispensing Systems with Mass spectrometry**; Gary J. Van Berkel[1]; Vilmos Kertesz[1]; Harry Boeltz[2]; *[1]Oak Ridge National Laboratory, Oak Ridge , TN; [2]Dispendix GmbH, Stuttgart, Germany*

2:30-4:30 pm Wednesday
FUNDAMENTALS: MOLECULAR MODELING AND QUANTUM MECHANICAL CALCULATIONS IN ION MOBILITY AND MS
Christopher Chouinard (PNNL)
Room 107-110 level 1

WOH pm 02:30 **Towards Small Molecule Unsupervised Structural Assignment Using TIMS-FT-ICR MS datasets**; Paolo Benigni[1]; Francisco Fernandez Lima[1]; *[1]Florida International University, Miami, FL*

WOH pm 02:50 **Advancements in Traveling Wave Ion Mobility Theory: Assessing the Conformational Heterogeneity of Proteins and Peptides in the Gas Phase**; Sugyan M Dixit[1]; Brandon T Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI*

WOH pm 03:10 ***De novo* Elucidation of Protein Structures with Ion Mobility Spectrometry / Mass Spectrometry**; Christian Bleiholder; *Florida State University, Tallahassee, FL*

WOH pm 03:30 **Integrative Mass Spectrometry Reveals the Conformational States of Protein Supercomplexes: Application to Cullin Ring Ligases in Complex with Cop9 Signalosome**; Andy Lau[1]; Zainab Ahdash[1]; Chloe Martens[1]; Carla Schmidt[2]; Argyris Politis[3]; *[1]King's College London, London, London; [2]Martin Luther University Halle-Wittenberg, Halle (Saale), Germany; [3]King's College London, UK*

WOH pm 03:50 **A Coarse-grained Computational Approach to Enable Structure Elucidation of Polymorphic Nucleic Acids by ion Mobility Mass Spectrometry**; Rebecca J D'Esposito[1]; Jennifer L Lippens[2]; Sweta Vangaveti[3]; Srivathsan Ranganathan[3]; Dan Fabris[1]; *[1]University at Albany-SUNY, Albany, NY; [2]Amgen, Thousand Oaks, CA; [3]The RNA Institute, Albany, NY*

WOH pm 04:10 **Molecular Dynamics Simulations of the Electrospray Process: Why Do Crown Ethers Suppress Protein Supercharging?**; Lars Konermann[1]; Haidy Metwally[2]; *[1]Univ. of Western Ontario, London, ON, Canada; [2]Univ. of Western Ontario, London, ON, Canada*

4:45-5:30 pm Wednesday
ASMS MEETING
Vicki Wysocki, ASMS President, presiding
Enjoy a beverage and hear the latest ASMS news.
Sagamore 5-7 level 2

5:45 - 7:00 PM WEDNESDAY WORKSHOPS

There are light refreshments in common areas.

01. Career and Collaboration Opportunities in China

Presiding: Yinsheng Wang, Andy Tao
Room 130

Recent economic development in China has created numerous job opportunities for postdoctoral fellows and graduate students with training in mass spectrometry. The overall objective of this workshop is to provide information to those individuals with interest in seeking job opportunities in China. We plan to invite 6-7 mass spectrometrists from academia, pharmaceutical companies, and instrument vendors in China as panel members for this workshop. These individuals will share with the participating graduate students and postdocs about their experiences and perspectives in finding jobs, establishing an independent research program in universities, hiring mass spectrometrists, and developing international collaborations in China. We believe that the workshop will benefit young and next-generation scientists in mass spectrometry by providing a unique perspective of job opportunities in China and assisting with their career development. The workshop will be mixed with panelist presentations and Q/A session with the participating students and postdocs.

02. High Spatial Resolution 2D and 3D Mass Spectrometry Analysis: New Trends

Presiding: Francisco Fernandez-Lima, Chistopher Anderton
Room 131-132

Recent advances on 2D and 3D Mass Spectrometry analysis has driven many technological advances in biological, biomedical, materials, environmental and forensic sciences. With the development of new and the incorporation of hyphenated techniques during 2D and 3D MS analysis, there is a need to further develop universal, analysis and data processing protocols; definitions; reference guidelines; standard reference materials; and inter-laboratory comparisons.

This first workshop will provide an overview of the main 2D and 3D MS technologies from experts in the field and will focus on generating further strategies to integrate existing and new technologies and researches in the area of 2D and 3D MS analysis.

A preliminary list of topics will include:

i. High spatial resolution MS analysis (How is defined the spatial for different MS techniques?);
ii. Applications in Material, Biological and Forensic Sciences;

iii. 3D MS analysis and depth profiling;
iv. Theoretical treatment and existing data processing tools (open source and commercial); and
v. Hyphenated 2D and 3D MS techniques.

The workshop encourages the participation and presentations of new investigators, postdocs and graduate students. A combination of short presentations (2-3 slides/group) from representatives of the 2D and 3D MS techniques, with a balance between academic, national laboratories and industrial researchers will be follow by an open discussion forum. One of the goals of this workshop is to gather researchers and enable the discussion towards the development of an interest group within the ASMS community to address these new scientific challenges.

03. Diversity and Outreach
Presiding: Benjamin Garcia, Rena Robinson
Room 133-134

This workshop will serve as the first open meeting of the ASMS Diversity and Outreach Working Group. At the 2016 ASMS Conference, a committee was assembled and met to outline potential initiatives for enhancing the diversity of our society. Here specifically at this workshop, we will have a series of mini-talks by scientists that besides describing exciting new science, will also focus on their personal journeys into their professional careers. These talks will lead into a Discussion Panel, so that attendees will have a chance to ask any questions to committee members about scientific research paths, career and life choices, applying for next level positions, etc. Lastly, time will also be allotted for discussion of the initiatives of the Diversity and Outreach Working Group, and to solicit feedback from the ASMS community. We hope this workshop will begin to lay down the networking foundations for scientists who are interested in Diversity and Outreach to connect other scientists at all career levels.

04. Galaxy-P in the Cloud: Proteomic Informatics on JetStream
Presiding: Tim Griffin, Pratik Jagtap Jeremy Fischer
Room 135-136

The Galaxy bioinformatics platform has emerged as a valuable workflow engine for MS-based proteomic informatics. Galaxy enables integration of disparate software tools to build sophisticated workflows for proteomic, and even multi-omic data analysis. An active and collaborative community of researchers, including the Galaxy for proteomics (Galaxy-P) team, continues to extend Galaxy for these applications.

To date, Galaxy-P has been primarily accessible to those who are experienced users of the Galaxy platform. To extend its reach to the greater community, implementation of proteomics software on more accessible and scalable infrastructure is needed.

To address this need, the Galaxy-P team has partnered with the JetStream cyberinfrastructure resource. Maintained at Indiana University and supported by the NSF, Jetstream is a production-level cloud computing resource open to the research community. JetStream supports Galaxy instances as one of its core bioinformatics software.

This workshop will provide participants background on JetStream, including instructions on how it can be accessed and the hardware and software resources available. A hands-on demonstration opportunity will also be provided, highlighting Galaxy-P software and workflows that have been made available on JetStream. Attendees will take away knowledge on how to access this resource and make use of it for their own MS-based proteomics informatics needs.

05. Food Safety & Authenticity: HRMS Applications
(Flavor, Fragrance & Foodstuff Interest Group)
Presiding: David Schroeder, Sara Kern
Room 137-138

Food, Flavor and Fragrance High Resolution Mass Spectrometry (HRMS) applications and developments discussion continuation. Food contaminant, pesticide, non-targeted analyte identification, and natural product authenticity strategies will be discussed.

06. Energy, Petroleum, and Biofuels: Challenges
(Energy Petroleum & Biofuels Interest Group)
Presiding: Mark Barrow, David Stranz
Room 139

Energy-related samples present a number of analytical challenges. Petroleum is a highly complex mixture and mass spectrometry remains at the forefront of methods for sample characterization. Petroleum derivatives, including fuels which include biofuel components, are also areas of growing interest. As a result, researchers are faced with a range of experimental considerations in order to acquire data of high quality. Samples may undergo extraction or separation procedures, such as SARA fractionation, as an initial step. The choice of solvents used during sample preparation and the selection of the ionization method will influence the sample profile. Chromatography and ion mobility may be employed as additional separation approaches, offering potential for structural information while also introducing a further need for optimization. Dynamic range and, for FTMS instruments, space-charge are two of the experimental considerations during data acquisition. With such areas in mind, the workshop will feature discussion of experimental challenges that influence data quality.

07. Undergraduate Research in Mass Spectrometry: Making the Most of It (Undergraduate Research in MS Interest Group)
Presiding: Jim Pesavento, Megan Gessel
Room 140

This panel discussion, aimed at undergraduate students and their mentors, will focus on helping undergraduate students leverage their undergraduate research experiences into successful scientific careers. Panelists will discuss their experiences applying to graduate school and transitioning to a graduate school research environment, as well as working in industrial labs.

08. Quantitative Glycomics and Glycoproteomics
Presiding: Yehia Mechref
Room 141-142

The correlations between protein glycosylation and many biological processes and diseases are increasing the demand for quantitative glycomic strategies, enabling sensitive monitoring of changes in the abundance and structure of glycans. This is currently attained through multiple strategies employing several analytical techniques, such as capillary electrophoresis, liquid chromatography, and mass spectrometry. Detection and quantification of glycans often involve labeling with ionic and hydrophobic reagents to enhance detections in spectroscopic and mass spectrometric measurements. Recently, labeling with stable isotopic reagents has also been presented as a very viable strategy enabling relative quantitation. The different strategies available for reliable and sensitive quantitative glycomics will be described and discussed in this workshop, including MS of naïve, permethylated and derivatized glycans. Quantiation through the addition of standards or isotopically labeled glycans will also be discussed. Additionally, quantitative glycomics through stable isotopic labeling will also be discussed, such as stable isotopic labeling by permethylation and reductive amination. Multiplexing quantitative glycomics employing permethylation, TMT reagents, and QUANTITY will be described and discussed.

09. Mass Spectrometry in GMP Environment: Aspects of System Qualification and Method Validation
Presiding: Gyorgy Vas
Room 143-144

The workshop will continue to discuss the aspects of cGMP compliant instrument qualification practices, was started last year. We will discuss recent best practice, industry and regulatory expectations of Mass Spectrometric Instrument Qualification in a cGMP environment. Different solutions will be discuss, how to handle -on a regulatory compliant manner- the lack of regulatory documents and guidance related to this field. This year we will extend the scope for method validation best practice.

Attendees are expected from instrument vendors, pharmaceutical and food industry and regulatory agencies.

10. Mass Spectrometry in the Developing World: Supporting Education and Research
Presiding: Kym Faull
Room 145

Students in developing nations learn about mass spectrometry from text books. They rarely if ever get to actually see one, and never get to use them. Old but working instruments that are replaced with new versions could be made available to Universities in developing countries to be used for research and teaching purposes. This would entail shipping, installation, training and maintenance which would all require funding and support. Some aspects of maintenance and training could probably be accomplished via Skype and email. The big questions is: Is this feasible? It would be a noble aspiration for ASMS to embrace. It would improve our relations with the developing world and perhaps provide an example for other organizations (e.g. the NMR Society, etc) to follow. The Presider will begin with a brief description of a personal experience that stimulated him to organize this workshop. This was a memorable experience that forged a lifelong and enduring friendship. All those interested are invited to join in a discussion on this topic.

11. Lipidomics Data Processing and Analyses: Software Tools (Lipids & Lipodomics Interest Group)
Presiding: Todd Mitchell, Eva Duchoslav
Room 231-234

One of the key issues in lipidomics experiments is the bottleneck created by the large amount of data generated. Growing awareness of this issue has seen many academics and MS vendors develop software dedicated to the processing and analysis of this data. With a rapidly growing choice of both commercial software and freeware it can be difficult deciding what software is best for your experiment. In this workshop a panel of advanced users and software developers will share their experience with a variety of lipid and lipidomics-compatible software platforms, focusing on capabilities, tips and tricks, and answer your questions on the where, when and how of lipid MS data processing tools.

12. Data Independent Acquisition Strategies for Quantitative Proteomics: The Challenges of Scaling Up to Meet Demand (Data Independent Acquisition Interest Group)
Presiding: Ben Collins, Isabell Bludau
Room 235-238

A basic aim of most proteomics studies is to obtain a protein matrix with quantitative values for multiple proteins across various conditions. Data independent acquisition (DIA) has recently emerged as a promising method to generate such matrices with deep proteome coverage (similar to DDA) and consistent detection and quantification across large sample cohorts (comparable to SRM/PRM methods). A growing number research goals in the life sciences explicitly require the analysis of large numbers of samples (e.g. perturbation/drug screens, genetic association analysis, clinical/biomarkers, ...). But how broad and how deep can we go? What challenges are being encountered when attempting to scale-up? This workshop aims to discuss the scalability of DIA based methods with respect to both the number of conditions being simultaneously analyzed and proteome coverage. We will discuss issues associated with scalability broadly in three categories: proteome coverage of the spectral library (only for peptide-centric scoring), error rate control on the level of protein detection, and quantification consistency across large and heterogeneous sample cohorts. The workshop will focus on introducing the most recent concepts addressing these aspects and further aims to discuss and develop ideas to ensure the reporting of high-quality protein quantification matrices.

13. Nucleic Acid-based Therapeutics: Structure Identification and Bioanalysis (Oligonucleotides and Nucleic Acids Interest Group)
Presiding: Laixin Wang, Sam Wainhaus
Room 239

Following small molecules and monoclonal antibodies, nucleic acid-based therapeutics have emerged to be the third major drug development engine in the pharmaceutical industry. Starting from antisense in 1990s, RNAi in 2000s to CIRSPR and mRNA in 2010s. The rise of nucleic acid based therapeutics has coincided with an explosion in the understanding of the genetic cause of diseases, and the growing desire for precision medicine. LC-MS/MS and LC-HRAM are playing critical roles in the structure characterization and quantitative analysis of nucleic acid molecules. This workshop will focus on the assay development of sensitive and specific assays for structure identification and bioanalysis of nucleic acid based therapeutics and their metabolites. Selected presentations will demonstrate the challenges and solutions during the method development and sample analysis. The remaining time will be spent discussing the pitfalls and tips and tricks in sample preparation, LC development and MS optimization.

14. Ion Mobility Spectrometry: Towards Standard Operating Procedures (Ion Mobility MS Interest Group)
Presiding: Stephen Valentine, Valérie Gabelica, Brian Clowers
Room 240-242

In contrast to the m/z ratio which depends on the analyte only, ion mobility fundamentally depends upon the interactions of analyte ions with neutral gas molecules. Measuring gas-phase ion mobility, although becoming widespread, is not yet routine. Given the growing user base and range of home-made and commercial instrumentation, there is a need for standard operating procedures (SOPs), reference materials and well-defined performance metrics to ensure the quality and utility of experiments. The ion mobility spectrometry interest group workshop will provide a forum to discuss (1) the core issues for developing SOPs for IMS and (2) the minimum reporting requirements for peer-reviewed publication and data sharing.

15. Bioanalysis of Biosimilars (Regulated Bioanalysis Interest Group)
Presiding: Dian Su, Jian Wang, Fabio Garofolo
Room 243-245

Biosimilars are not exact duplicates of Innovator Biotherapeutics. Hence, the Regulatory Agency requirements for Biosimilars differ from those of small molecules. One important difference is the required evaluation of “similarity” of the Biosimilar compared to the innovator Biotherapeutic. Bioanalysis of Biosimilars is subject to endogenous interference, requiring specific and selective assay to ensure data reliability. The specificity and selectivity of traditional quantification approaches (Ligand Binding Assays - LBA) are dependent on the interaction of critical reagents to the Biotherapeutic. It is possible that the Innovator and the Biosimilar do not have the same binding characteristics towards the assay critical reagents. In this case, two assays with different critical reagents may be needed and the demonstration of biocomparability may be more complicated. LC-MS/MS and more recently HRMS have shown to be a successful technique for the Bioanalysis of Biotherapeutics. Unlike traditional approaches, LC-MS/MS and HRMS assays can be developed for the Bioanalysis of Biosimilars without using critical reagents and therefore only a single assay is needed for both Biosimilar and Innovator comparison. Experts in the field will share their experience in this highly interactive workshop.

AFTER 8:00 pm
CORPORATE HOSPITALITY SUITES
JW MARRIOTT HOTEL

From 6:45 am Thursday
CORPORATE BREAKFAST SEMINARS
Convention Center
Detailed schedule on page 15.
Pre-registration recommended, space is limited

8:30-10:30 am Thursday
INFORMATICS: INNOVATIONS
Dan Spellman (Merck & Co.)
Hall D level 1

ThOA am 08:30 **QCloud: A Cloud-based Quality Control System for the Proteomics Community**; Cristina Chiva[1,2]; Roger Olivella[1,2]; Eva Borràs[1,2]; Guadalupe Espadas[1,2]; Olga Pastor[1,2]; Amanda Solé[1,2]; Eduard Sabidó[1,2]; *[1]Proteomics Unit, Centre de Regulació Genòmica (CRG), Barcelona Institute of Science and Technology (BIST), Dr. Aiguader 88, Barcelona, Spain; [2]Universitat Pompeu Fabra (UPF), Dr. Aiguader 88, Barcelona, Spain*

ThOA am 08:50 **Paradigm Change in *de novo* Identification of Small Molecules: Giant Spectral Trees**; Tim J. Stratton[1]; Jakub Mezey[2]; Alena Bednarikova[2]; Andrea Belicova[2]; Jana Semanova[2]; Robert Mistrik[2]; *[1]ThermoFisher, San Jose, CA; [2]HighChem, Bratislava, Slovakia*

ThOA am 09:10 **Novoquest: Algorithm for *de novo* Sequencing of Cyclic Peptide Antibiotics Using Tandem Mass Spectrometry**; Bahar Behsaz[1]; Hosein Mohimani[1]; Pieter C. Dorrestein[1]; William Gerwick[1]; Pavel Pevzner[1]; *[1]University of California, San Diego, La Jolla, CA*

ThOA am 09:30 **Software for Proteome Dynamics from Metabolic Labeling and LC-MS**; Mahbubur Rahman[1]; Takhar Kasumov[2]; Rovshan Sadygov[3]; *[1]UTMB, Galveston, TX; [2]Northeast Ohio Medical Univeristy, Rootstown, OH; [3]University of Texas, Galveston, TX*

ThOA am 09:50 **Visualizing Flux Between Proteoforms Implicated in Stress Response by Constructing and Quantifying Proteoform Families**; Anthony J. Cesnik[1]; Michael R. Shortreed[1]; Leah V. Schaffer[1]; Brian L. Frey[1]; Rachel A Knoener[1]; Mark Scalf[1]; Stefan K Solntsev[1]; Lloyd M. Smith[1]; *[1]University of Wisconsin Madison, Madison, WI*

ThOA am 10:10 **PeptideExplorer: A Repository-scale Intuitive Navigation Interface over Millions of Identifications**; Benjamin Pullman[1]; Jeremy Carver[1]; Mingxun Wang[1]; Nuno Bandeira[1,2]; *[1]Computer Science and Engineering Department, UC San Diego, San Diego, CA; [2]Skaggs School of Pharmacy, University of California San Diego, La Jolla, CA*

8:30-10:30 am Thursday
MS IN THE QC LAB
Izabella Sokolowska (Janssen Research & Development)
500 Ballroom level 1

ThOB am 08:30 **Quantitation of Capsaicinoids by UPLC/MS using Single Quadrupole Mass Spectrometry in the QC Environment**; Jane E. Guido; *Kalsec, Inc., Kalamazoo, MI*

ThOB am 08:50 **LC Peak Purity Assessment Using a Novel LC-MS Data Processing Approach**; Adrien Nyakas[1]; Agron Selami[1]; Hannes Patrik Plattner[1]; Dirk Bächle[1]; *[1]Bachem AG, Bubendorf, Switzerland*

ThOB am 09:10 **Mass Spectrometry Applications in Medical Cannabis Contamination Testing**; Scott Kuzdzal[1]; Bob Clifford[1]; Jeff Dahl[2]; Dan Davis[1]; Nicole Lock[3]; Paul Winkler[2]; Julie Kowalski[4]; Jason Zitzer[5]; Derek Laine[5]; *[1]Shimadzu Scientific Instr., Columbia, MD; [2]Shimadzu Scientific Instruments, Columbia, MD; [3]Shimadzu Scientific Instruments, Somerset, NJ; [4]Restek Corporation, Bellefonte, PA; [5]Trace Analytics, Spokane, WA*

ThOB am 09:30 **Adding Mass Spectrometry Capabilities to LC/UV-based Workflows as Part of Lifecycle Management in the Routine Analysis of Small Biotherapeutics**; Ximo Zhang[1]; Robert Birdsall[1]; Brooke M Koshel[1]; Joe Fredette[1]; Min Du[1]; Ying Qing Yu[1]; *[1]Waters Corporation, Milford, MA*

ThOB am 09:50 **Development and Validation of a LC-MS Glycosylation Method for Testing of a Monoclonal Antibody Product Containing Two Glycosylation Sites**; Zhirui Lian[1]; Angelia Reed-Bogan[1]; Eric Adamec[1]; Bryan Harmon[1]; Haiyan Lu[1]; Bereket Yemane[1]; Jean Yang[1]; Roujian Zhang[1]; *[1]Eli Lilly and Company, Indianapolis, IN*

ThOB am 10:10 **Automated Data Processing for Quality Monitoring of Biotherapeutics by Multi-attribute Methods (MAMs)**; Joe Shambaugh[1]; Stefano Gotta[2]; David Bush[1]; Maurizio Bronzetti[1]; Cassandra Wigmore[2]; *[1]Genedata Inc, Lexington, MA; [2]Genedata AG, Basel, Switzerland*

8:30-10:30 am Thursday
MEMBRANE PROTEIN MS
Julian Whitelegge (UCLA)
Sagamore 1-3 level 2

ThOC am 08:30 **Native MS Reveals Lipid-dependent Dimer Formation for the Eukaryotic Purine symporter UapA**; Euan Pyle[1]; Bernadette Byrne[2]; Argyris Politis[3]; *[1]Imperial College London and King's College London, London, UK; [2]Imperial College London, London; [3]King's College London, London*

ThOC am 08:50 **Collision Induced Unfolding Reveals the Regiospecific Ligand Binding Behavior of Integral Membrane Translocator Protein (TSPO)**; Sarah Fantin[1]; Shuai Niu[1]; Jian Liu[2]; Richard A Kerr[1]; Shelagh M Ferguson-Miller[2]; Brandon T Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI; [2]Michigan State University, Lansing, MI*

ThOC am 09:10 **FT-ICR MS as a *bona-fide* Platform for Multimeric Membrane Protein Characterization** ; Jennifer L. Lippens[1]; Michael Nshanian[2]; Pascal F Egea[2]; Joseph A Loo[2]; Iain D G Campuzano[1]; *[1]Amgen, Newbury Park, CA; [2]UCLA, Los Angeles, CA*

ThOC am 09:30 **Automated Proteoform Elucidation of Chromatographically Resolved Hyper-Modified Intrinsically Disordered Membrane Proteins**; Daniel A Plymire[1]; John R Corbett[1,2]; Casey E Wing[1]; William S Phipps[1]; Steven M Patrie[1,2]; *[1]University of Texas Southwestern Medical Center, Dallas, TX; [2]University of Texas at Dallas, Richardson, TX*

ThOC am 09:50 **Mapping the Orientation and Sites of Neurosteroid Photolabeling in the Ion Channel, Glic Using Top-Down, Middle-Down, and Bottom-Up Mass Spectrometry**; Wayland WL Cheng[1]; Zi-Wei Chen[1]; Melissa M Budelier[1]; Douglas F Covey[1]; Gustav Akk[1]; Evers S Alex[1]; *[1]Washington University in St. Louis, Saint Louis, MO*

ThOC am 10:10 **Studying the Structural Dynamics of the Eukaryotic Neurotransmitter Transporter dDAT by Hydrogen/Deuterium Exchange Mass Spectrometry**; Anne Kathrine Nielsen[1,2]; Ingvar R Möller[2]; Kasper D Rand[2]; Claus J Loland[1]; *[1]Department of Neuroscience and Pharmacology, University of Copenhagen, Copenhagen, Denmark; [2]Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark*

8:30-10:30 am Thursday
NUCLEIC ACIDS AND OLIGONUCLEOTIDES
Kym Faull (UCLA)
Sagamore 4 level 2

ThOD am 08:30 **Advances in LC-MS of Oligonucleotides**; Michael G. Bartlett[1]; Babak Basiri[2]; *[1]University of Georgia, Athens, GA; [2]University of Georgia, Athens, GA*

ThOD am 08:50 **Analysis of Global RNA Mononucleoside Modifications by nanoLC-MS/MS**; Kevin A. Janssen[1]; Ranran Wu[1]; Benjamin A. Garcia[1]; *[1]Epigenetics Institute, University of Pennsylvania Perelman School of Medicine, Philadelphia, PA*

ThOD am 09:10 **Multiplex Analysis of Oligonucleotides and RNA Digestion Products through polyA Polymerase (PAP) with Azido-Modified NTP Labeling**; Kayla Borland[1]; Patrick A. Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH*

ThOD am 09:30 **System Wide Elucidation of the Dynamics of Proteins Associating with Single Messenger RNAs (mRNAs)**; Erica Jacobs[1]; Peter C Fridy[1]; Michael P Rout[1]; Brian T Chait[1]; *[1]Rockefeller University, New York, NY*

ThOD am 09:50 **Real-time Monitoring of Nucleic Acid Dynamics by ESI-MS Melting Experiments**; Botros Toro[1]; Pan T.X. Li[1]; Daniele Fabris[1]; *[1]SUNY at Albany, Albany, NY*

ThOD am 10:10 **Multi-omic Mass Spectrometry Applications: Dozens of tRNA Modifications and an Alternative Genetic Code Control Dormancy and Antibiotic Resistance in Mycobacteria**; Weiling Maggie Cai[1]; Yok Hian Chionh[1]; Nicholas Davis[2]; Jennifer Hu[2]; Thomas Begley[3]; Peter Dedon[1, 4]; *[1]Singapore-MIT Alliance for Research and Technology, Infectious Disease IRG, Singapore, Singapore; [2]Massachusetts Institute of Technology, Cambridge, MA; [3]3SUNY Polytechnic Institute, Albany, NY; [4]Massachusetts Institute of Technology, Cambridge, MA*

8:30-10:30 am Thursday
NATIVE MS IN STRUCTURAL BIOLOGY
Frank Sobott (University of Antwerp)
Sagamore 5-7 level 2

ThOE am 08:30 **Probing Structure and Capturing Transient Intermediates by Monitoring Reactions of Protein Assemblies in Real Time by High-Resolution Native Mass Spectrometry**; Paul Dominic B. Olinares[1]; Virapat Kieuvongngam[2]; Natalia Orlova[3]; Julio C Padovan[1]; David Jeruzalmi[3]; Jue Chen[2]; Brian T Chait[1]; *[1]Laboratory of Mass Spectrometry and Gaseous Ion Chemistry, The Rockefeller University, New York, NY; [2]The Rockefeller University and Howard Hughes Medical Institute, New York, NY; [3]Department of Chemistry and Biochemistry, City College of New York, New York, NY*

ThOE am 08:50 **Structural Characterization of Protein-Lipid Complexes Involved in Clathrin-Mediated Endocytosis**; Johannes Heidemann[1]; Maria M. Garcia Alai[2]; Anna Gieras[2]; Rob Meijers[2]; Charlotte Uetrecht[1, 3]; *[1]Heinrich Pette Institute, Hamburg, Germany; [2]EMBL, Hamburg, Germany; [3]XFEL GmbH, Hamburg, Germany*

ThOE am 09:10 **The Molecular Clock of Islet Amyloid Polypeptide: from Dimerization to Deamidation**; Yuko P. Y. Lam[1]; Christopher A. Wootton[1]; Juan Wei[1]; Ian Hands-Portman[1]; Mark P. Barrow[1]; Peter B. O'Connor[1]; *[1]University of Warwick, Coventry, UK*

ThOE am 09:30 **Structural Transitions of Brome Mosaic Virus Tracked by Charge Detection Mass Spectrometry**; Kevin M Bond[1]; Irina B Tsvetkova[1]; Bogdan Dragnea[1]; Martin F Jarrold[1]; *[1]Indiana University Bloomington, Bloomington, IN*

ThOE am 09:50 **Investigation of Protein-Protein Interactions using Surface Induced Dissociation - Mass Spectrometry**; Stacey Nash[1]; Florian Busch[1]; Kristina Heyn[2]; Fabian Ruperti[2]; Rainer Merkl[2]; Reinhard Sterner[2]; Vicki Wysocki[1]; *[1]The Ohio State University, Columbus, OHIO; [2]Institute of Biophysics and Physical Biochemistry, University of Regensburg, Regensburg, Germany*

ThOE am 10:10 **Double Mutant Cycles in the Gas Phase: Measuring Inter-protein Pairwise Interaction Energies from a Single Native Mass Spectrum**; Jelena Cveticanin[1]; Miri Sokolovski[2]; Deborah Hayoun[1]; Amnon Horovitz[2]; Michal Sharon[1]; *[1]Department of Biomolecular Sciences, Weizmann Institute Of Science, Rehovot, Israel; [2]Department of Structural Biology, Weizmann Institute of Science, Rehovot, Israel*

8:30-10:30 am Thursday
IMAGING: PHARMACEUTICALS, METABOLITES, AND LIPIDS
Andreas Römpp (University of Bayreuth)
Wabash level 1

ThOF am 08:30 **A Multimodal Imaging Approach to Characterize Intramuscular and Subcutaneous Drug Depots of Cabotegravir**; Reid Groseclose[1]; Fang Xie[1]; Beat Jucker[1]; Hasan Alsaid[1]; Manish Gupta[1]; Stephen Castellino[1]; *[1]GlaxoSmithKline, King of Prussia, PA*

ThOF am 08:50 **Drug Localization at the Single Cell Level - A Multimodal Mass Spectrometry Imaging Approach**; Neda Najafinobar[1]; Lena von Sydow[1]; Mike J. Hickey[1]; Chad S. Elmore[1]; Michael E. Kurczy[1]; Magnus Klarqvist[1]; Tineke Papavoine[2]; Per Malmberg[3]; *[1]Astrazeneca, Mölndal, Mölndal; [2]AstraZeneca R&D, Gothenburg, Sweden; [3]Chalmers University of Technology, Gothenburg, Sweden*

ThOF am 09:10 **Spatial Single-cell Metabolomics of Monolayer Cell Cultures with 10 um Resolution**; Luca Rappez[1]; Bachir El Debs[1]; Andrew Palmer[1]; Artem Tarasov[1]; Vitaly Kovalev[1]; Ivan Protsyuk[1]; Mira Stadler[2]; Prasad Phapale[1]; Megan Stanifer[2]; Joel Selkrig[1]; Mathias Heikenwälder[2]; Steeve Boulant[2]; Nassos Typas[1]; Theodore Alexandrov[1, 3]; *[1]EMBL, Heidelberg, Heidelberg; [2]German Cancer Research Center (DKFZ), Heidelberg, Germany; [3]Skaggs School of Pharmacy, University of California San Diego, La Jolla, CA*

ThOF am 09:30 **Characterization of Diet-induced Molecular Changes in Ovarian Reserves of Aedes aegypti Using 3D-MSI-TOF-SIMS and MALDI FT-ICR MS**; Anthony Castellanos[1]; Quentin Vanbellingen[2]; Paolo Benigni[2]; Veronika Michalkova[2]; Marcela Nouzova[2]; Fernando Noriega[2]; Francisco Fernandez-Lima[2]; *[1]Florida International University, Miami, FL; [2]Florida International University, Miami, FL*

ThOF am 09:50 **Molecular Insights of the Song Learning Behaviour of Zebra Finch during Ontogeny with Multimodal Mass Spectrometry Imaging**; Nina Ogrinc Potocnik[1]; Julie Hamaide[2]; Tiffany Porta[1]; Garima Yadav[2]; Arnoud Prop[1]; Annemie van der Linden[2]; Ron MA Heeren[1]; *[1]M4i Institute, Division of Imaging Mass Spectrometry, Maastricht University, Maastricht, Netherlands; [2]Bio-Imaging Lab, University of Antwerp, Wilrijk, Belgium*

ThOF am 10:10 **Three-Dimensional MALDI MSI Reveals Distinct Metabolic Compartments and Unique Metabolite Distributions in Soybean Root Nodules**; Dusan Velickovic[1]; Beverly Agtuca[2]; Sylwia Stopka[3];

Akos Vertes[3]; David W. Koppenaal[1]; Ljiljana Pasa-Tolic[1]; Gary Stacey[2]; Christopher R Anderton[1]; *[1]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Earth and Biological Sciences Directorate, Richland, WA; [2]Divisions of Plant Sciences and Biochemistry, C. S. Bond Life Sciences Center, University of Missouri, Columbia, MO; [3]Department of Chemistry, W. M. Keck Institute for Proteomics Technology and Applications, The George Washington University, Washington, DC*

8:30-10:30 am Thursday
GC/MS, GC/GC/MS, GC/MS/MS, AND GC/HRMS
Tom Doherty (Agilent)
Room 101-106 level 1

ThOG am 08:30 **Comprehensive Steroid Analysis by GCxGC-TOFMS**; Michael Groessl[1]; Andrea Bileck[1]; Sofia Verouti[1]; Genevieve Escher[1]; *[1]University Hospital Bern, Bern, Switzerland*

ThOG am 08:50 **Application of Py-GCxGC/MS Combined with Chemometrics for the Elucidation of Ancient East Asian Papermaking Materials**; Bin Han[1]; Jérome Vial[2]; Masamitsu Inaba[3]; Michel Sablier[1]; *[1]Sorbonne Universités, Centre de Recherche sur la Conservation (CRC, USR 3224), Muséum national d'Histoire naturelle, Ministère de la Culture et de la Communication, CNRS, Paris, France; [2]Department of Analytical, Bioanalytical Sciences and Miniaturization (LSABM), Institute of Chemistry, Biology and Innovation (CBI)–ESPCI ParisTech, CNRS UMR 8231, Paris, France; [3]Conservation Science Laboratory, Graduate School of Conservation, Tokyo Geijutsu Daigaku, Taito-ku, Japan*

ThOG am 09:10 **Shifting the Paradigm in Gas Chromatography Mass Spectrometry Pesticide Analysis by High Resolution Mass Spectrometry**; Samanta Uclés[1]; Ana Lozano[1]; Francisco José Díaz-Galiano[1]; Amadeo R. Fernández-Alba[1]; *[1]European Union Reference Laboratory for Pesticide Residues in Fruit & Vegetables, ALMERÍA, Spain*

ThOG am 09:30 **GC-QTOFMS and GC-MS/MS with EI and CI as Highly Versatile Platforms for Metabolomics and Metabolic Flux Analysis in Biotechnology**; Teresa Mairinger[1, 2]; Christina Troyer[1]; Wolfhard Wegscheider[3]; Juergen Zanghellini[1, 2]; Diethard Mattanovich[1, 2]; Gunda Koellensperger[4]; Stephan Hann[1, 2]; *[1]BOKU-Vienna, Vienna, Austria; [2]Austrian Centre of Industrial Biotechnology, Vienna, Austria; [3]Montanuniversitaet Leoben, Leoben, Austria; [4]University of Vienna, Vienna, Austria*

ThOG am 09:50 **GC-MS with Cold EI for Improved Sample Identification**; Aviv Amirav[1]; Alexander B. Fialkov[1]; Uri Keshet[1]; Tal Alon[1]; *[1]Tel Aviv University, Tel Aviv, Israel*

ThOG am 10:10 **Data Quality Assurance Methods for Seized-Drug Mass Spectral Libraries**; Weihua Ji[1]; William E. Wallace[1]; Dmitrii V. Tchekhovskoi[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD*

8:30-10:30 am Thursday
FUNDAMENTALS FOR EVERYONE
Nick Polfer (University of Florida)
Room 107-110 level 1

ThOH am 08:30 **Mass Resolution, Mass Resolving Power, Mass Accuracy, and Mass Calibration: State of the Art and Future Prospects**; Alan G. Marshall[1, 2]; Lissa C Anderson[1]; Greg T Blakney[3]; Yuri E Corilo[3]; Ryan P Rodgers[3, 4]; Donald F Smith[3]; Chad R Weisbrod[3]; Christopher L Hendrickson[3, 4]; *[1]Ion Cyclotron Resonance Program, NHMFL, Tallahassee, FL; [2]Dept. of Chemistry & Biochemistry, Florida State University, Tallahassee, FL; [3]ICR Program, NHMFL, Tallahassee, FL; [4]Dept of Chemistry Biochemistry, Florida State University, Tallahassee, FL*

ThOH am 08:50 **How to Reconstruct Collision Cross Section Distributions from Arrival Time Distributions measured in Drift Tube IMS**; Adrien Marchand[1]; Sandrine Livet[1]; Solenne Delahaye[1]; Frédéric Rosu[2]; Valérie Gabelica[1]; *[1]University of Bordeaux, Pessac, FR; [2]IECB, Bordeaux, France*

ThOH am 09:10 **Mechanistic Insights Gained from Spontaneous Ionization Using Solid or Solvent Matrices**; Charles N. Mcewen[1, 2]; Madeline A. Fenner[1]; Khoa Hoang[1]; Milan Pophristic[2]; *[1]Univ. of the Sciences, Philadelphia, PA; [2]MSTM, LLC., Newark, DE*

ThOH am 09:30 **Can Electrospray Ionization Tolerate High Concentrations (100+ mM) of Nonvolatile Salts?**; Anna C. Susa[1]; Zijie Xia[1]; Evan R. Williams[2]; *[1]University of California, Berkeley, Berkeley, CA; [2]University of California, Berkeley, Berkeley, CA*

ThOH am 09:50 **How Hot are Your Ions Really? Experimental Measurements of the Bond Energies of Benzylpyridinium "Thermometer" Ions**; John E Carpenter[1]; Christopher P. McNary[1]; April Furin[1]; Andrew Sweeney[1]; Peter B. Armentrout[1]; *[1]University of Utah, Salt Lake City, UT*

ThOH am 10:10 **Making Ions Shine with Mass Spectrometry and UV/vis Spectroscopy: Powerful Potential and Potential Pitfalls**; Rebecca A. Jockusch[1]; Sydney M.J. Wellman[2]; Martin F. Czar[2]; Stephen V. Sciuto[2]; *[1]University of Toronto, Toronto, ON, Canada; [2]University of Toronto, Toronto, ON, Canada*

10:30 am-2:30 pm Thursday
THURSDAY POSTER SESSION
Poster/Exhibit Hall
Lunch concessions are open 11:00 am-2:00 pm
Odd-number posters present 10:30 am-1:00 pm
Even-number posters present 12:00-2:30 pm

2:30-4:30 pm Thursday
INFORMATICS: DISCOVERY PROTEOMICS
Masaru Miyagi (Case Western University)
Hall D

ThOA pm 02:30 **The Spectra-Cluster Toolsuite: Enhancing Proteomics Analysis Through Spectrum Clustering**; Johannes Griss[1, 2]; Juan Antonio Vizcaino[2]; *[1]Medical University of Vienna, KIMCL, Vienna, No State/Province; [2]EMBL-EBI, Cambridge, Cambridgeshire*

ThOA pm 02:50 **Illuminating the "Dark Matter" of Shotgun Proteomics Using MSFragger**; Andy Kong[1]; Dmitry M. Avtonomov[1]; Felipe Leprevost[1]; Dattatreya Mellacheruvu[1]; Alexey Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI*

ThOA pm 03:10 **Discovery of Fusion Peptides through Bottom-Up Proteomic Analysis Using Separate b and y-Ion Databases**; Zach Rolfs[1]; Stefan K. Solntsev[1]; Michael R. Shortreed[1]; Brian L. Frey[1]; Mark Scalf[1]; Alan D. Attie[1]; Lloyd M. Smith[1]; *[1]University of Wisconsin-Madison, Madison, WI*

ThOA pm 03:30 **Mango: A General Search Tool for CID-cleavage Cross-linked Peptide Identification**; Jared P. Mohr[1]; Poorna Perumalla[1]; Juan D. Chavez[1]; Jimmy K Eng[1]; James E. Bruce[1]; *[1]University of Washington Genome Sciences, Seattle, WA*

ThOA pm 03:50 **Predicting Kinase-Substrate Associations Using Patterns of Co-Phosphorylation**; Marzieh Ayati[1]; Danica Wiredja[2]; Daniela Schlatzer[2]; Sean Maxwell[2]; Mehmet Koyuturk[1, 2]; Mark R. Chance[2]; *[1]Case Western Reserve University, Cleveland, OH; [2]Center for Proteomics and Bioinformatics, Case Western Reserve University, Cleveland, OH*

ThOA pm 04:10 **Network Discovery of Chronologically Conserved Proteome Dynamics between the Cells and the Tissues**; Mahbubur Rahman[1]; Rovshan Sadygov[1]; *[1]UTMB, Galveston, TX*

2:30-4:30 pm Thursday
HRMS FOR QUANTITATION IN DRUG DISCOVERY, DEVELOPMENT AND BEYOND
Martha Stapels (Sanofi)
500 Ballroom level 1

ThOB pm 02:30 **High Mass Analysis and Signal Processing on an FT-ICR: From Native Monoclonal Antibodies to Antibody Drug Conjugates and Beyond**; Iain D G Campuzano[1]; Steve Van Orden[2]; Huilin Li[3]; David Kilgour[4]; Jennifer L Lippens[1]; Michael Nshanian[3]; Chawita Netirojjanakul[1]; Piriya Wongkongkathep[3]; Pascal F Egea[3]; Joseph A Loo[3]; *[1]Amgen Inc., Thousand Oaks, CA; [2]Bruker Daltonic, Billerica, MA; [3]University of California, Los Angeles, Los Angeles, CA; [4]Nottingham Trent University, Nottingham, UK*

ThOB pm 02:50 **Discovery of Sequence Variants during IgG1 Monoclonal Antibody Cell Line Selection by High-throughput LC-MS Analysis**; Yan Wang[1]; Chongfeng Xu[1]; Zoran Sosic[1]; Li Zang[1]; *[1]Biogen, Cambridge, MA*

ThOB pm 03:10 **Role of Copper Incorportation from CuATSM in the Turnover of SOD1 in ALS Mouse Models**; Joe Beckman[1]; Blaine Roberts[2]; Valery G. Voinov[3]; Yury Vasil'ev[3]; *[1]Oregon State University, Corvallis, OR; [2]Florey Institute of Neuroscience, Melbourne, Australia; [3]e-MSion, Corvallis, OR*

ThOB pm 03:30 **ETD and CID MS/MS Analysis at 21 T and X-Ray Crystallography Define Structural Differences in Variants of 45 kDa Proteins**; Lissa Anderson[1]; Maria Håkansson[2]; Björn Walse[2]; Carol Nilsson[3, 3]; *[1]NHMFL, Tallahassee, FL; [2]SARomics Biostructures AB, Lund, Sweden; [3]Lund University, Lund, Sweden*

ThOB pm 03:50 **High Resolution Mass Spectrometry towards Targeted Residual CHO Protein Quantification**; Matt Schenauer[1]; Doug Rehder[1]; Darren Brown[1]; *[1]Gilead Sciences, Oceanside, CA*

ThOB pm 04:10 **Understanding the Metabolism of the Anticancer Drug Triapine Using Electrochemistry AND Liquid Chromatography Coupled to Mass Spectrometry (EC/LC/MS)**; Karla Pelivan[1]; Lisa Frensemeier[2]; Uwe Karst[2]; Gunda Koellensperger[3]; Petra Heffeter[4]; Walter Berger[4]; Christian Kowol[1]; Bernhard Keppler[1]; *[1]Institute of Inorganic Chemistry, Faculty of Chemistry, University of Vienna, Vienna, Austria; [2]Institute of Inorganic and Analytical Chemistry, University of Muenster, Muenster, Germany; [3]Institute of Analytical Chemistry, Faculty of Chemistry, University of Vienna, Vienna, Austria; [4]Institute of Cancer Research, Medical University of Vienna, Vienna, Austria*

2:30-4:30 pm Thursday
TOP DOWN PROTEIN ANALYSIS
Brandon Rutolo (University of Michigan)
Sagamore 1-3 level 2

ThOC pm 02:30 **Top-Down Mass Spectrometry of Large Proteins up to 223 kDa Enabled by Serial Size Exclusion Chromatography**; Trisha Tucholski[1]; Wenxuan Cai[1]; Bifan Chen[1]; Andrew J Alpert[2]; Samantha Knott[1]; Ying Ge[1]; *[1]University of Wisconsin, Madison, Madison, WI; [2]PolyLC Inc., Columbia, MD*

ThOC pm 02:50 **Autopiquer - New Developments in Robust Peak Picking for Mass Spectra**; David P. A. Kilgour[1]; Anton N. Kozhinov[2]; Konstantin O. Nagornov[2]; Samantha L. Kilgour[3]; Manuela Tosin[3]; Sam Hughes[4]; Colin Logan Mackay[4]; Magnus Palmblad[5]; David J. Clarke[4]; David Boocock[1]; Yury O. Tsybin[2]; *[1]Nottingham Trent University, Nottingham, UK; [2]Spectroswiss Sàrl, Lausanne, Switzerland; [3]University of Warwick, Coventry, UK; [4]University of Edinburgh, Edinburgh, UK; [5]Leiden University Medical Center, Leiden, Netherlands*

ThOC pm 03:10 **Characterization of Surface Induced Dissociation (SID) as a Top-Down Fragmentation Technique**; Alyssa Q. Stiving[1]; Joshua D. Gilbert[1]; Vicki H. Wysocki[1]; *[1]The Ohio State University, Columbus, OH*

ThOC pm 03:30 **Elucidation of Combinatorial Post Translational Modifications (PTMs) of Histones via Top-Down Analysis Using 193 nm Ultraviolet Photodissociation (UVPD)**; Sylvester Greer[1]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

ThOC pm 03:50 **Developments in Instrumentation and Data Acquisition Methods for Top-down 21 T FT-ICR Proteomics**; Lissa C. Anderson[1]; Chad R. Weisbrod[1]; Nathan K. Kaiser[1]; Greg T. Blakney[1]; Christopher L. Hendrickson[1, 2]; Alan G. Marshall[1, 2]; *[1]Ion Cyclotron Resonance Program, NHMFL, Tallahassee, FL; [2]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL*

ThOC pm 04:10 **The Omni-trap: A New Processing Cell Equipped with an Extensive Arsenal of Ion Activation Techniques for Top-down Mass spectrometry**; Dimitris Papanastasiou[1]; Diamantis Kounadis[2]; Alexander Lekkas[2]; Andreas Bozatzidis[2]; Ioannis Orfanopoulos[2]; Emmanuel Raptakis[2]; Maria Reinhardt-Szyba[3]; Eugen Damoc[3]; Alexander Makarov[3]; Roman Zubarev[4]; *[1]Fasmatech, Athens, Attiki; [2]Fasmatech Science & Technology, Athens, Greece; [3]Thermofisher, Bremen, Bremen; [4]Karolinska Institute, Stockholm , Uppland*

2:30-4:30 pm Thursday
CARBOHYDRATES
Brad Bendiak (University of Colorado HSC)
Sagamore 4 level 2

ThOD pm 02:30 **Glycoanalysis with Cold Ion Spectroscopy and Ion Mobility: Study of Glycosaminoglycans and Human Milk Oligosaccharides**; Neelam Khanal[1]; Chiara Masellis[2]; Michael Z. Kamrath[2]; David E Clemmer[1]; Thomas R. Rizzo[2]; *[1]Indiana University, Bloomington, IN; [2]EPFL, Lausanne, Switzerland*

ThOD pm 02:50 **Disentangling Carbohydrate Isomer Mixtures via Combination of Metal Ion Binding, Gas-Phase Ion Chemistry, Tandem Mass Spectrometryand Ion Mobility Spectrometry**; Katherine Schumacher[1]; Eric D. Dodds[1]; *[1]University of Nebraska - Lincoln, Lincoln, NE*

ThOD pm 03:10 **Electronic Excitation Dissociation Characterization of Native Glycans Derivatized with a Reducing-End Fixed Charge**; Yang Tang[1]; Yi Pu[1]; Catherine E. Costello[1]; Cheng Lin[1]; *[1]Boston University, Boston, MA*

ThOD pm 03:30 **Identifying Carbohydrate Isomers via an Ion/Molecule Reaction with Water**; Matthew T. Campbell[1]; Gary L. Glish[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC*

ThOD pm 03:50 **An Integrated Capillary Electrophoresis-Mass Spectrometry Platform for the Analysis of Glycosaminoglycan Mixtures**; Patience Sanderson[1]; Morgan Stickney[2]; Franklin E Leach III[2]; James Xia[3]; Yanlei Yu[4]; Fuming Zhang[5]; Robert J Linhardt[4]; Jonathan I Amster[2]; *[1]University of Georgia, Athens, GA; [2]University of Georgia, Athens, GA; [3]CMP Scientific, Corp., Brooklyn, NY; [4]Rensselaer Polytechnic Institute, Troy, NY; [5]Rensselaer Polytechnic Institute, Troy, NY*

ThOD pm 04:10 **Cationized Carbohydrate Fragmentation Chemistry: Influence of Glycosidic Linkage Position and Stereochemistry**; Benjamin Bythell[1]; Jordan M Rabus[1]; Maha T. Abutokaikah[1]; *[1]University of Missouri-St. Louis, St. Louis, MO*

2:30-4:30 pm Thursday
PROTEIN-LIGAND INTERACTIONS
Robert Cole (Johns Hopkins University)
Sagamore 5-7 level 2

ThOE pm 02:30 **Novel Methodology for Pulldown of RNA-Binding Proteins and Application to let-7 miRNAs**; Lisa Jenkins[1]; Genevieve Di Tomasso[2]; Pascale Legault[2]; *[1]National Cancer Institute, Bethesda, MD; [2]Université de Montréal, Montréal, QC, Canada*

ThOE pm 02:50 **Improved Identification of Ligand Binding Sites in Integral Membrane Proteins**; Melissa M Budelier[1]; Wayland W.L Cheng[1]; Zi-Wei Chen[1]; Douglas F Covey[1]; James W Janetka[1]; Alex S Evers[1]; *[1]Washington University, St Louis, MO*

ThOE pm 03:10 **On Chip Interaction Proteomics for Low Input Protein Samples**; Cristina Furlan[1]; René A.M. Dirks[1]; Peter Thomas[2]; Robert C. Jones[2]; Hendrik Marks[1]; Michiel Vermeulen[1]; *[1]Radboud University, Nijmegen; [2]Fluidigm Corporation, South San Francisco, CA*

ThOE pm 03:30 **Native Top-Down Mass Spectrometry used for the Characterization of Novel Metal Binding by Endogenous Proteins and Complexes**; Nicole A. Haverland[1]; Owen S. Skinner[1]; Luca Fornelli[1]; Areeba A. Tariq[1]; Luis F. Schachner[1]; Philip D. Compton[1]; Neil L. Kelleher[1]; *[1]Northwestern University, Evanston, IL*

ThOE pm 03:50 **Contributions of Individual Ligands to the Structural Stability of an Iron Binding Protein During an Unfolding Transition**; Daniel W. Woodall[1]; Tarick J. El-Baba[1]; Wen Liu[2]; Yang Liu[2]; Arthur Laganowsky[2]; David E. Clemmer[1]; *[1]Indiana University, Bloomington, IN; [2]Texas A&M University, College Station, TX*

ThOE pm 04:10 **Online Monitoring of Enzymatic Reactions Using Time-Resolved Desorption Electrospray Ionization Mass Spectrometry**; Hao Chen[1]; Si Cheng[1]; Qiuhua Wu[1]; *[1]Ohio University, Athens, OH*

2:30-4:30 pm Thursday
IMAGING: BIOMEDICAL APPLICATIONS
Troy Wood (SUNY Buffalo)
Wabash level 1

ThOF pm 02:30 **Tumor Margin Determination during Neurosurgery using DESI**; R. Graham Cooks [1]; Valentina Pirro[2]; Clint Miles Alfaro[2]; Alan Jarmusch[2]; Eyas M Hattab[3]; Aaron A Cohen-Gadol[4]; *[1]Purdue University, West Lafayette , IN; [2]Purdue University, West Lafayette, IN; [3]Indiana University, Bloomington, IN; [4]Indiana University−Purdue University, Indianapolis, IN*

ThOF pm 02:50 **Predicting ER, PR, and HER2 Status in Breast Cancer Using Metabolic Markers by DESI-MS Imaging**; Kyana Garza[1]; Raquel Mary Rodrigues Peres[2]; Andréia M Porcari[2]; Jialing Zhang[1]; Jonathan Young[1]; Robert J. Tibshirani[3]; Geisilene Russano de Paiva[2]; Wendong Yu[4]; Chandandeep Nagi[4]; Marcos N. Eberlin[2]; Luis O. Zanatta Sarian[2]; Livia S. Eberlin[1]; *[1]University of Texas at Austin, Austin, TX; [2]State University of Campinas, Campinas, Brazil; [3]Stanford University, Stanford, CA; [4]Baylor College of Medicine, Houston, TX*

ThOF pm 03:10 **Molecular and Elemental Mass Spectrometry Imaging of Photosensitizers in Human Brain Tumors after Fluorescence-guided Resection**; Sabrina Kröger[1]; Ann-Christin Niehoff[1]; Astrid Jeibmann[2]; Walter Stummer[3]; Uwe Karst[1]; *[1]University of Münster, Institute of Inorganic and Analytical Chemistry, Münster, Germany; [2]University Hospital of Münster, Institute of Neuropathology, Münster, Germany; [3]University Hospital of Münster, Department of Neurosurgery, Münster, Germany*

ThOF pm 03:30 **Building an Accurate Model of the Invasive Tumor Microenvironment with Colon Carcinoma Three Dimensional Tumor Spheroids**; Eric M. Weaver[1]; Pinar Zorlutuna[1, 2]; Amanda B. Hummon[1, 3]; *[1]Harper Cancer Research Institute, University of Notre Dame, Notre Dame, IN; [2]Department of Aerospace and Mechanical Engineering, Bioengineering Graduate Program University of Notre Dame, Notre Dame, IN; [3]Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN*

ThOF pm 03:50 **Mapping Non-alcoholic Fatty Liver Disease Progression with Mass Spectrometry Imaging**; Zoe Hall[1]; Nicholas J Bond[1]; Tom Ashmore[1]; Julian L Griffin[1]; *[1]Department of Biochemistry, University of Cambridge, Cambridge, UK*

ThOF pm 04:10 **Characterization of Single Fluorescent Motor Neurons in Amyotrophic Lateral Sclerosis (ALS) Mouse Brains via MALDI Mass Spectrometry Imaging (MSI)**; Catherine M. Rawlins[1]; David Calligaris[2]; Jared R. Auclair[1]; April J. Harry[1, 3]; Kylie A. Bemis[1]; Ed Luther[1]; Olga Vitek[1]; Nathalie Y.R. Agar[2]; Jeffrey N. Agar[1]; *[1]Northeastern University, Boston, MA; [2]Brigham and Women's Hospital, Harvard Medical School, Boston, MA; [3]Purdue University, West Lafayette, IN*

2:30-4:30 pm Thursday
INSTRUMENTATION: INNOVATIVE SEPARATIONS APPROACHES COUPLED TO MS
Mary Wirth (Purdue University)
Room 101-106 level 1

ThOG pm 02:30 **A Method and a Hyphenated to Mass Spectrometry Device for Isolation, Detection and Quantification of Abnormal Proteoforms in blood**; Roman Zubarev; *Karolinska Institute, Stockholm , Uppland*

ThOG pm 02:50 **Discovery Bottom-up Proteomic Characterization for Limited Populations of Neurons by Ultrasensitive CE-nanoESI-MS**; Sam Choi[1]; Marta Zamarbide[1]; M. Chiara Manzini[1]; Peter Nemes[2]; *[1]George Washington University, Washington, DC; [2]George Washington University, Washington , DC*

ThOG pm 03:10 **Chip-Based Capillary Electrophoresis Mass Spectrometry (CE/MS) for Rapid Intact Mass and Structure Analysis for Large and Small Molecules**; Tawnya Flick[1]; Laura Blue[2]; Shawn Pope[2]; J. Scott Mellors[3]; *[1]Amgen Inc., Thousand Oaks, California; [2]Amgen, Thousand Oaks, CA; [3]908 Devices Inc., Boston, MA*

ThOG pm 03:30 **An MS Based Rapid Alternative to Western Blotting**; Fred Regnier[1]; Jinhee Kim[2]; Christian Vukas[2]; *[1]Purdue University / Novilytic, Carmel, IN; [2]Novilytic LLC, West Lafayette, IN*

ThOG pm 03:50 **Accumulation and Compression of Billions of Ions Using CRIMP in SLIM Significantly Improves Sensitivity and Ion Mobility Resolution**; Liulin Deng[1]; Sandilya Garimella[1]; Ahmed Mohamed Hamid[1]; Ian K Webb[1]; Xueyun Y Zheng[1]; Roza Wojcik[1]; Spencer A Prost[1]; Gordon A Anderson[1]; Erin S Baker[1]; Yehia M Ibrahim[1]; Richard D. Smith[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

ThOG pm 04:10 **Analysis of Proteins, Protein Complexes and Protein-Ligand Interactions using Size Exclusion Chromatography-High Resolution Mass Spectrometry**; Aniruddha Sahasrabuddhe[1]; Florian Busch[1]; Zachary VanAernum[1]; Brian Rivera[2]; Vicki Wysocki[1]; *[1]The Ohio State University, Columbus, OH; [2]Phenomenex, Inc., Torrance, CA*

2:30-4:30 pm Thursday
ENERGY, PETROLEUM, AND BIOFUELS: INSTRUMENTATION AND APPLICATIONS
Ryan Rodgers (National High Magnetic Field Lab)
Room 107-110

ThOH pm 02:30 **High-temperature GC×GC with 70eV EI and 10.5eV SPI Nominal and High-resolution TOFMS for the Characterization of Heavy Petroleum Matrices**; Maximilian Jennerwein[1, 2]; Uwe Kaefer[2, 3]; Ralf Zimmermann[2, 3]; Juergen Wendt[4]; Thomas Wilharm[1]; Thomas Groeger[3]; *[1]ASG Analytik Service-Gesellschaft mbH, Neusäss, Germany; [2]Joint Mass Spectrometry Centre / Chair of Analytical Chemistry, University of Rostock, Rostock, Germany; [3]Joint Mass Spectrometry Centre / Cooperation Group Comprehensive Molecular Analytics, Helmholtz Zentrum München, Neuherberg, Germany; [4]LECO European Application & Technology Centre, Berlin, Germany*

ThOH pm 02:50 **Understanding the Structural Space of Hydrocarbons in Crude Oil Using TIMS-FT-ICR MS**; Paolo Benigni[1]; Mark E. Ridgeway[2]; Melvin A Park[2]; Francisco Fernandez-Lima[1, 3]; *[1]Florida Intl University, Miami, FL; [2]Bruker Daltonics, Billerica, MA; [3]Biomolecular Sciences Institute, Miami, FL*

ThOH pm 03:10 **Application of Selective Labeling Reactions to Explore Structure of Fossil Humic Substances by FT ICR MS**; Alexander Zherebker[1, 2]; Yury Kostyukevich[2, 3, 4]; Alexey S Kononikhin[2, 4, 5]; Oleg Kharybin[3]; Irina V Perminova[1]; Eugene (Evgeny) Nikolaev[2, 3, 4, 5]; *[1]Lomonosov Moscow State University, Department of Chemistry, Moscow, Russia; [2]Institute for Energy Problems of Chemical Physics of RAS, Moscow, Russia; [3]Skolkovo Institute of Science and Technology, Skolkovo, Russia; [4]Emanuel Institute of Biochemical Physics of Russian Academy of Sciences, Moscow, Russia; [5]Moscow Institute of Physics and Technology (State University), Dolgoprudnyj, Russia*

ThOH pm 03:30 **Rapid Characterization of Polyalphaolefins Using Atmospheric Pressure Photoionization and Atmospheric Solid Analysis Probe Coupled to Ion Mobility - Mass Spectrometry**; Anna Luiza Mendes Siqueira[1, 2]; Mathieu Beaumesnil[1, 2]; Corinne Loutelier-Bourhis[2]; Carlos Afonso[2]; Amandine Racaud[1]; *[1]TOTAL Marketing & Services, Research Center, Solaize, France; [2]Normandie Univ., UNIROUEN, INSA Rouen, CNRS, COBRA, Rouen, France*

ThOH pm 03:50 **Composition Analysis of Aviation Fuels and Fuel Additives for Rational Development of Renewable Aviation Fuels**; Katherine Wehde[1]; Mark Romanczyk[1]; Petr Vozka[2]; Jorge Ramirez Velasco[3]; Rodney Trice[3]; Gozdem Kilaz[2]; Hilkka Kenttamaa[1]; *[1]Department of Chemistry, Purdue University, West Lafayette, IN; [2]Department of Aviation Technology, Purdue University, West Lafayette, IN; [3]Department of Materials Engineering, Purdue University, West Lafayette, IN*

ThOH pm 04:10 **Complementarity of ESI, APPI and LDI FT-ICR MS Analyses for the Comprehensive Description of Raw and Deoxygenated Pyrolysis Bio-oils**; Jasmine Hertzog[1]; Vincent Carré[1]; Liangyuan Jia[2]; Yann Le Brech[2]; Ludovic Pinard[3]; Colin Logan Mackay[4]; Ondřej Mašek[5]; Anthony Dufour[2]; Frédéric Aubriet[1]; *[1]LCP-A2MC - Université de Lorraine, Metz, France; [2]LRGP - Université de Lorraine, Nancy, France; [3]IC2MP - Université de Poitiers, Poitiers, France; [4]School of Chemistry - University of Edinburgh, Edinburgh, UK; [5]UK Biochar Research Center - University of Edinburgh, Edinburgh, UK*

4:45-5:30 pm Thursday
PLENARY LECTURE
Richard A. Yost (University of Florida)
Hall D level 1

Saving the Great Coral Reefs

Kristen Marhaver
Research Station Carmabi

6:30-9:00 pm Thursday
CLOSING EVENT
INDIANA STATE MUSEUM
Advance purchase ticket is required ($30).

ODD-NUMBERED POSTERS PRESENT 10:30 AM - 1:00 PM. EVEN-NUMBERED POSTERS PRESENT 12:00 - 2:30 PM.

MONDAY POSTERS

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

TUESDAY POSTERS

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

ODD-NUMBERED POSTERS PRESENT 10:30 AM - 1:00 PM. EVEN-NUMBERED POSTERS PRESENT 12:30 - 2:30 PM.

WEDNESDAY POSTERS

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

THURSDAY POSTERS

Set up all Thursday posters ..... 7:30 – 8:00 am
Odd-numbered posters present ..... 10:30 am – 1:00 pm
Even-numbered posters present ..... 12:00 – 2:30 pm
Remove all Thursday posters ..... 2:30 – 3:00 pm

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

AMBIENT IONIZATION: FUNDAMENTALS AND INSTRUMENTATION
001 - 016

MP 001 **Exploration of Mixed-gas Flowing Atmospheric-Pressure Afterglow as an Atmospheric Pressure Chemical Ionization and Photoionization Source for Mass Spectrometry**; Sunil Badal[1]; Jessica Hellinger[1]; Jacob Shelley[1]; *[1]Department of Chemistry and Chemical Biology, Rensselaer Polytechnic Institute, Troy, NY*

MP 002 ***In-vivo* Endoscopic Mass Spectrometry with Moving String as Sampling Probe**; Lee Chuin Chen; *University of Yamanashi, Kofu, Yamanashi*

MP 003 **Multi-mode Reactive Nano-electrospray Ion Source for Droplet Chemistry using Picoliter Samples**; Dmytro Kulyk[1]; Abraham K. Badu-Tawiah[2]; *[1]The Ohio State University, Columbus, Ohio; [2]The Ohio State University, Columbus, OH*

MP 004 **Ambient Nanoparticle and Plasma Assisted Laser Desorption Ionization Mass Spectrometric Methods (Ambient nanoPALDI MS) for Live Tissue Analysis**; Jae Young Kim[1]; Eun Seok Seo[1]; Hyunmin Kim[2]; Dong-Kwon Lim[3]; Dae Won Moon[1]; *[1]Department of New Biology, DGIST, Daegu, South Korea; [2]Division of Nano and Energy Convergence Research, DGIST, Daegu, South Korea; [3]KU-KIST Graduate School of Converging Science and Technology, Korea University, Seoul, South Korea*

MP 005 **Ambient Chemical Analysis of Biological Tissues by the Combination of Extractive Electrospray Ionization Mass Spectrometry with High-Frequency Resonance Field Desorption**; Vladimir Frankevich[1]; Vitaliy V Chagovets[1]; Xinchen Wang[2]; Alisa Tokareva[1]; Alexey S Kononikhin[1]; Konstantin Chingin[2]; Huanwen Chen[2]; Gennady Sukhikh[1]; *[1]Federal State Budget Institution "Research Center for Obstetrics, Gynecology and Perinatology" Ministry of Healthcare of the Russian Federation, Moscow, Russia; [2]Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, East China University of Technology, Nanchang, China*

MP 006 **Innovations in Liquid Microjunction Surface Sampling Probe Mass Spectrometry**; Louis Searcy[1]; Arun Wanchoo[2]; Cuong Nguyen[2]; Timothy J. Garrett[2]; Richard A Yost[2]; *[1]University of Florida, Gainesville, FL; [2]University of Florida, Gainesville, FL*

MP 007 **Multimodal Imaging Combining Fluorescence Microscopy and Laser Ablation Electrospray Ionization Mass Spectrometry**; Sylwia A Stopka[1]; Beverly J Agtuca[2]; Christopher R Anderton[3]; Rikkita Khattar[1]; David W Koppenaal[3]; Ljiljana Pasa-Tolic[3]; Gary Stacey[2]; Akos Vertes[1]; *[1]George Washington University, Washington, DC; [2]University of Missouri, Columbia, MO; [3]Pacific Northwest National Laboratory, Richland, WA*

MP 008 **Development of a Continuous Flow Infrared MALDESI Source for Online LC/MS Analysis of Peptides and Proteins**; Koichi Kimura[1]; Hisanao Hazama[1]; Kunio Awazu[1, 2, 3]; *[1]Graduate School of Engineering, Suita, Japan; [2]Graduate School of Frontier Biosciences, Suita, Japan; [3]Global Center for Medical Engineering and Informatics, Osaka University, Suita, Japan*

MP 009 **Analytical Validation of a Portable MS System Featuring Interchangeable, Ambient Ionization Sources during Field Operation**; Shahnaz Mukta[1]; Zachary E. Lawton[1]; William L. Fantigante[1]; Herbert Oberacher[2]; Christopher C. Mulligan[1]; *[1]Illinois State University, Normal, IL; [2]Innsbruck Medical University, Innsbruck, Austria*

MP 010 **Compact Laser Ablation Microwave Plasma Ionization for Ambient Molecular and Atomic Analysis**; Gaston D. Merideth II[1]; Kelsey R. May[1]; Kenyon Evans-Nguyen[1]; *[1]The University of Tampa, Tampa, FL*

MP 011 **Novel Ambient Ionization Source for Real-Time Breath Analysis**; Michael Wei[1]; Christopher Gongar[1]; Michael Costanzo[2]; Jared Boock[3]; Richard A. Yost[1]; *[1]University of Florida, Gainesville, FL; [2]Breathtec Biomedical, Inc., Gainesville, Florida; [3]Cannabix Technologies, Gainesville, FL*

MP 012 **Theta Emitters for Fast Mixing: Hydrogen-Deuterium Exchange, Ion Form**; Zijie Xia[1]; Evan R. Williams[1]; *[1]University of California, Berkeley, Berkeley, CA*

MP 013 **Coated Blade Spray: Shifting the Paradigm of Direct Sample Introduction to Mass Spectrometry**; German Augusto Gomez-Rios[1]; Marcos Tascon[1]; Nathaly Reyes Garces[1]; Daniel Rickert[1]; Ezel Boyaci[1]; Justen J Poole[1]; Karol Jaroch[2]; Barbara Bojko[1, 2]; Janusz Pawliszyn[1]; *[1]University of Waterloo, Waterloo, Ontario; [2]Nicolaus Copernicus University in Torun, Bydgoszcz, Poland*

MP 014 **Molecularly Imprinted Membrane Electrospray Ionization for Direct Sample Analyses**; Mei Zhang; *Chinese CDC, Beijing, China*

MP 015 **Comparison of the Novel UniSpray Ion Source to A Range of Alternative Atmospheric Pressure Ionization Sources**; Eleanor Riches[1]; G. John Langley[2]; Julie M. Herniman[2]; *[1]Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK; [2]Faculty of Natural and Environmental Sciences, Chemistry, University of Southampton, Highfield, UK*

MP 016 **Develpoment and Testing of a Simple, Low-Cost Low-Temperature Plasma Ionization Source**; Clinton A. L. McFeely[1]; Victoria Zelikson[1]; Scott Gronert[1]; *[1]Virginia Commonwealth University, Richmond, VA*

ANTIBODIES & ANTIBODY DRUG CONJUGATES I
017 - 027

MP 017 **Accurate Mass Determination of Intact Monoclonal Antibody Charge Variants, Including Deamidation Products, using CZE-CZE-QqTOF-MS**; Kevin Jooß[1, 2]; Jens Hühner[1, 3]; Christian Neusüß[1]; *[1]Aalen University of Applied Sciences, Aalen, Germany; [2]Helmholtz Zentrum München, Neuherberg, Germany; [3]University of Tübingen, Tübingen, Germany*

MP 018 **Robust and Sensitive Workflow for Qualitative and Quantitative Analysis of Intact Monoclonal Antibodies Using Microflow LC and TripleTOF Mass Spectrometry**; Gavin Fischer; *Redwood City*

MP 019 **Analysis of Bispecific mAb by Size Exclusion Chromatography and Mass Spectrometry** ; Keegan Gike[1]; Atis Chakrabarti[1]; *[1]Tosoh Bioscience LLC, King of Prussia, PA*

MP 020 **Charge Heterogeneity Analysis of Intact Monoclonal Antibodies using CESI-MS**; Esme Candish[1]; Christopher Loessner[2]; Stephen J. Lock[3]; Olga Friese[4]; Elaine Stephens[5]; Jason C. Rouse[5]; Bryan Fonslow[1]; *[1]SCIEX, Brea, CA; [2]SCIEX, Darmstadt, Germany; [3]SCIEX, Warrington, UK; [4]Biotherapeutics Pharm. Sci., Pfizer Inc., St. Louis, MO; [5]Biotherapeutics Pharm. Sci., Pfizer Inc., Andover, MA*

MP 021 **Manipulation of Chromatographic Conditions to Maximize the LC/MS Effectiveness**; Suresh Babu Cv[1]; Ning Tang[2]; Anne Blackwell[3]; *[1]Agilent Technologies , Bangalore , Karnataka; [2]Agilent Technologies, Santa Clara, CA; [3]Agilent Technologies, Wilmington, DE*

MP 022 **A Quick and Simple Approach for Confirmation of Isomerization and Racemization of Aspartate in Asp-Asp Motifs of a Therapeutic Protein**; Weitao Jia[1]; Xiaoxiao Liu[1]; Jennifer Zhang[1]; *[1]Genentech, Inc, South San Francisco, CA*

MP 023 **High-throughput Mass Spectrometric Analysis: From Covalently Labeled Proteins to Antibody Drug Conjugates**; Chawita Netirojjanakul[1]; Iain D. G. Campuzano[1]; Tisha San Miguel[1]; Aiko Umeda[1]; Jason Long[1]; *[1]Amgen, Thousand Oaks, CA*

MP 024 **High Resolution LC/MS Separation and Characterization of Chemoenzymatic Site-specific Engineered Antibody-Drug Conjugates (ADCs)**; Shanhua Lin[1]; Terry Zhang[2]; Brian Agnew[3]; Jonathan Josephs[2]; Xiaodong Liu[4]; *[1]Thermo Fisher Scientific, Sunnyvale, CA; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Eugene, OR; [4]Thermo Fisher Scientific, Sunnyvale, CA*

MP 025 **Development of a High-Throughput Workflow to Characterize Bispecific Antibody Variants**; Michael Bacica[1]; Yaqiong Lin[1]; Jing Zhuo[1]; Marissa M Horn[1]; Karen J Froning[1]; Jonathan Fittchett[1]; Bryan E. Jones[1]; *[1]Lilly Research Labs, San Diego, CA*

MP 026 **Characterization of Monoclonal Antibodies and Antibody Drug Conjugates using Microfluidic CE-MS Technology**; Erin Redman[1]; Joshua P. Guerrette[1]; Michael P. Goodwin[2]; J. Scott Mellors[1]; *[1]908 Devices, Inc., Carrboro, NC; [2]908 Devices Inc., Boston, MA*

MP 027 **A Novel Capillary Isoelectric Focusing - Mass Spectrometry (cIEF-MS) Technique for Monoclonal Antibody Charge Variants Analysis**; Jun Dai[1]; Yingru Zhang[2]; Fahim Sarah Zarrin[3]; Rena Wang[3]; James Xia[3]; Wayne Heacock[4]; Dat Phan[4]; Dawn Stickle[4]; John Sausen[4]; *[1]Bristol-Myers Squibb, Princeton, NJ; [2]Bristol-Myers Squibb, Princeton, NJ; [3]CMP Scientific, Corp., Brooklyn, N.Y.; [4]Agilent Technologies, Inc., Wilmington, DE*

BIOMARKERS: DISCOVERY I
028 - 050

MP 028 **Tumor Specific Signature Pathway Showing Differentially Expressed Proteins in Prostate Cell Lines using Proteomics Approach**; Arum Park[1]; Jiyeong Lee[2]; Sora Mun[1]; Doo Jin Kim[2]; Byung Heun Cha[2]; YuRim Lee[4]; Tag Keun Yoo[3]; Hee-Gyoo Kang[1, 2]; *[1]Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Seongnam, South Korea; [2]Department of Biomedical Laboratory Science, College of Health Science, Eulji University, Seongnam, South Korea; [3]Department of Urology, College of Medicine, Eulji University, Daejeon, South Korea; [4]Eulji University, Seongnam-si, South Korea*

MP 029 **Rheumatoid Factor-Correlated Proteins are Useful Screening Markers for Autoimmune and Infectious Diseases with Rheumatoid Factor**; Sora Mun[1]; Doojin Kim[2]; Jiyeong Lee[2]; Arum Park[1]; AeEun Seok[1]; Yeon-Tae Chun[2]; Hee-Gyoo Kang[1, 2]; *[1]Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Seongnam-si, South Korea; [2]Department of Biomedical Laboratory Science, College of Health Sciences, Eulji University, Seongnam-si, South Korea*

MP 030 **Disease-specific IgG Fc N-glycosylationas Personalized Biomarkers to Differentiate Lung Cancer from Benign Lung Diseases**; Dan Zhang[1]; Tianjing Chen[1]; Mo Zhang[1]; Zhili Li[1]; *[1]Institute of Basic Medical Sciences, CAMS & PUMC, Beijing*

MP 031 **Deep Proteome Profiling of Extracellular Vesicles Isolated from Human Plasma**; Ole Østergaard[1, 2]; Christian D. Kelstrup[2]; Julia T. Tanassi[1]; Niels H. H. Heegaard[1, 3]; Jesper V. Olsen[2]; *[1]Statens Serum Institut, Copenhagen, Denmark; [2]Novo Nordisk Foundation Center for Protein Research, Faculty of Health Sciences, University of Copenhagen, Copenhagen, Denmark; [3]Department of Clinical Biochemistry and Pharmacology, Odense University Hospital, Odense, Denmark*

MP 032 **Collagen Proteins in Colorectal Liver Metastasis**; Nick A. van Huizen[1]; Robert R.J. Coebergh van den Braak[1]; Michael Doukas[1]; Lennard J.M. Dekker[1]; Theo M. Luider[1]; Jan N.M. IJzermans[1]; *[1]Erasmus MC, Rotterdam, Zuid-Holland*

MP 033 **Abundant Protein Depletion of Human Plasma Samples – A Reproducibility and Scaling Study**; Sergei Snovida[1]; Katherine E. Herting[2]; Ramesh Ganapathy[2]; Ryan Bomgarden[2]; Barbara J. Kaboord[2]; Chris Etienne[2]; John C. Rogers[2]; *[1]Thermo Fisher Scientific, Rockford, IL; [2]ThermoFisher Scientific, Rockford, IL*

MP 034 **Assessment of Neopterin as a Potential Biomarker of Beta Cell Function in Human Urine Utilizing UPLC-MS/MS**; Kimberly A Navetta[1]; Jennifer Colangelo[2]; *[1]Pfizer Inc., Groton, CT; [2]Pfizer Inc, Groton, CT*

MP 035 **Proteomic Characterization of Laser Microdissected Myometrium and Trophoblast Compartments in Placenta Accreta**; Brian L. Hood[1]; Rebecca A. Keller[2]; Guisong Wang[1]; Julie Oliver[1]; Melinda M. Sanders[3]; Xiaohong Wang[3]; Alfred Khoury[4]; William A. Campbell[2]; Chad A. Hamilton[1, 5]; George L. Maxwell[1, 4, 6]; Thomas P. Conrads[1, 6]; *[1]Women's Health Integrated Research Center, Gynecologic Cancer Center of Excellence, Annandale, VA; [2]Division of Maternal-Fetal Medicine, Department of Obstetrics & Gynecology, University of Connecticut School of Medicine, Farmington, CT; [3]Department of Pathology and Histology, University of Connecticut School of Medicine, Farmington, CT; [4]Department of Obstetrics & Gynecology, Inova Fairfax Hospital, Falls Church, VA; [5]Gynecologic Oncology Service, Walter Reed National Military Medical Center, Bethesda, MD; [6]Inova Schar Cancer Institute, Falls Church, VA*

MP 036 **Dramatic Alterations in RNA Binding and Exosome-Associated Proteins Occur in Breast Cancer as Revealed by Proteomic Analysis of FFPE tissue**; Ten-Yang Yen [1]; Moe Thein[1]; Roger Yen[1]; Bruce A. Macher[1]; Leslie C. Timpe[1]; *[1]San Francisco State University, San Francisco , CA*

MP 037 **Identification of Peptides from Dehalococcoides mccartyi Protein Biomarkers in Chloroethene Contaminated Groundwater Samples through a Standard-Free LC-MRM-MS Approach**; Manuel Villalobos[1, 2]; Cynthia M. Swift[1, 2]; Karuna Chourey[2]; Frank Löffler[1]; Robert L. Hettich[1, 2]; *[1]University of Tennessee, Knoxville, TN; [2]Oak Ridge National Lab, Oak Ridge, TN*

MP 038 **Lipidomic Analysis of CSF from Patients with Neoplastic Meningitis (NM): A Pilot Study Identifying Biomarkers for Early Detection of NM**; Shinji K. Strain[1]; Morris D. Groves[2]; Mark R. Emmett[1, 3, 4, 5, 6]; *[1]Department of Neuroscience and Cell Biology, University of Texas Medical Branch, Galveston, TX; [2]Austin Brain Tumor Center, Texas Oncology/US Oncology Research, Austin, TX; [3]Department of Biochemistry and Molecular Biology, University of Texas Medical Branch, Galveston, TX; [4]Department of Pharmacology and Toxicology, University of Texas Medical Branch, Galveston, TX; [5]Department of Radiation Oncology, University of Texas Medical Branch, Galveston, TXuni; [6]UTMB Cancer Center, Galveston, TX*

MP 039 **Epidermal Lipids Detected by Multiple Reaction Monitoring (MRM)-profiling as Potential Biomarkers for Atopic Dermatitis**; Jackeline Franco[1]; Christina R. Ferreira[2]; Tiago José Paschoal Sobreira[2]; John P Sundberg[3]; Harm HogenEsch[4]; *[1]Purdue University, West Lafayette, IN; [2]Bindley Bioscience Center, Purdue University, West Lafayette, IN; [3]The Jackson Laboratory, Bar Harbor, MN; [4]Purdue University, West lafayette, IN*

MP 040 **Reproducible Single Shot Plasma Proteome Profiling with High Throughput Capabilities on a Robust Capillary Flow Setup**; Roland Bruderer[1]; Oliver M. Bernhardt[1]; Tejas Gandhi[1]; Sebastian Mueller[1]; Polina Mironova[2]; Ondine Walter[2]; Jérôme Carayol[2]; Jörg Hager[2]; Armand Valsesia[2]; Loïc Dayon[2]; Jan Muntel[1]; Arne Astrup[3]; Wim H.R. Saris[4]; Lukas Reiter[1]; *[1]Biognosys, Zurich, Switzerland; [2]Nestlé Institute of Health Sciences, Lausanne, Switzerland; [3]University of Copenhagen, Copenhagen, Denmark; [4]Maastricht University Medical Centre, Maastricht, Netherlands*

MP 041 **Identification of Predictive Biomarkers of Doxorubicin-induced Clinical Cardiotoxicity**; Li-Rong Yu[1]; Jaclyn R Daniels[1]; Zhijun Cao[1]; Jinchun Sun[1]; Richard D Beger[1]; Issam Makhoul[2]; Suzanne Klimberg[2]; Jeanne Wei[2]; Valentina K Todorova[2]; *[1]National Center for Toxicological Research, FDA, Jefferson, AR; [2]University of Arkansas for Medical Sciences, Little Rock, AR*

MP 042 **Assessment of the Effects of Pollutants in the Great Lakes on the Human Proteome**; Emmalyn Dupree[1]; Bernard Crimmins[2]; Thomas Holsen[2]; James Pagano[3]; Brooke Thompson[4]; Krista Christensen[4]; Michelle Raymond[4]; Costel C Darie[5]; *[1]Biochemistry and Proteomics Group, Department of Chemistry and Biomolecular Science, Clarkson University, Potsdam, NY; [2]Department of Civil and Environmental Engineering, Clarkson University, Potsdam, NY; [3]Department of Chemistry, SUNY Oswego, Oswego, NY; [4]Wisconsin Department of Health Services, Madison, WI; [5]Biochemistry & Proteomics Group, Department of Chemistry & Biomolecular Science, Clarkson University, Potsdam, NY*

MP 043 **Development of a Mass Spectrometry-Based Targeted Quantitative Assay for use in the Identification of a Colorectal Cancer Peptide Signature**; Jia You[1]; Athit Kao[1]; Roslyn Dillon[1]; Lisa J. Croner[1]; John E. Blume[1]; Ryan W. Benz[1]; Bruce E. Wilcox[1]; *[1]Applied Proteomics Inc., San Diego, CA*

MP 044 **Nitroproteome Analysis of a Model of Acute Kidney Injury from Renal Ischemia/Reperfusion**; Pamella Araujo Malagrino[1]; Gabriela Venturini[2]; Rafael Dariolli[2]; Kallyandra Padilha[2]; Tamiris Gois[2]; Karina Morais Cardozo[3]; Valdemir Melechco Carvalho[3]; Jessica Silva Salgueiro[3]; Jose Eduardo Krieger[2]; Alexandre Costa Pereira[2]; *[1], São Paulo, São Paulo; [2]Heart Institute, Sao Paulo, SP; [3]Fleury Group, Sao Paulo, Brazil*

MP 045 **In-quest of Biomarkers for Early Diagnosis of Alzheimer's Disease using LC-QTOF-MS/MS Based Lipidomics**; Chandana Mannem[1]; Jagan A. Pillai[2]; Christine Reece[2]; Yan Xu[1, 3]; *[1]Department of Chemistry, Cleveland State University, Cleveland, OH; [2]Luo Ruvo Center for Brain Health, Cleveland Clinic, Cleveland, OH; [3]Case Comprehensive Cancer Center, Case Western Reserve University, Cleveland, OH*

MP 046 **A Study of Label-Free and Isobaric Tag Approaches for the Detection of Biologically Relevant Changes in PAX8 Overexpressed MOSE Cells**; Melissa R Pergande[1]; Laura R Hardy[1]; Carol Haney-Ball[2]; Vadiraja Bhat[3]; Joanna E Burdette[1]; Stephanie M Cologna[1]; *[1]University of Illinois at Chicago, Chicago, IL; [2]Agilent Technologies, Inc., Santa Clara, CA; [3]Agilent Technologies, Inc., Wilmington, DE*

MP 047 **Use of Phosphoproteomics in Human Induced Pluripotent Stem Cell-Derived Cardiomyocytes for Investigation of Cardiac Toxicity of HCV-NS5B Antivirus Drugs**; Zhenlian Ke Tracy[1]; John Imredy[1]; Edward Lis[1]; Bharathi Balasubramanian[1]; Raymond Gonzalez[1]; *[1]Merck & Co., West Point, PA*

MP 048 **Use of Tyr-kinase Inhibitors to Identify Cross-Talk between Signaling Pathways and Novel Protein Drug-Targets**; Iulia M. Lazar[1]; Nicole Smith[1]; *[1]Virginia Polytechnic Institute & State University, Blacksburg, VA*

MP 049 **Temporal Effects of Novel Combinatorial Chemotherapeutics on Pancreatic Cancer Cells Investigated via Large-scale, Ion-Current Based Quantitative Proteomics**; Xue Wang[1, 2]; Jin Niu[1]; Jun Li[1]; Xiaomeng Shen[3]; Shichen Shen[1]; Robert M Straubinger[1, 2]; Jun Qu[1, 2]; *[1]University at Buffalo, Buffalo, NY; [2]Roswell Park Cancer Institute, Buffalo, NY; [3]Amgen, South San Francisco, CA*

MP 050 **Dried Matrix Spots Sampling in LC-MS Based Non-Targeted Proteomics – What Can You Expect from Different Sampling Materials and Devices?**; Cecilie Rosting[1]; Astrid Gjelstad[1]; Trine Grønhaug Halvorsen[1]; *[1]School of Pharmacy, University of Oslo, Oslo, Norway*

BIOMOLECULAR STRUCTURE ANALYSIS: CHEMICAL CROSSLINKING AND COVALENT LABELING I
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MP 051 **Proteome-wide Identification of Protein-Protein Interactions by *in-vivo* Chemical Crosslinking and Mass Spectrometry**; Elena L. Rudashevskaya[1]; Tomáš Ječmen[1]; Karl A.T. Makepeace[2, 3]; Jason J. Serpa[2]; Yassene Mohammed[2, 4]; Evgeniy V. Petrotchenko[2]; Chris Meisinger[5]; Rene Zahedi[1]; Albert Sickmann[1]; Christoph H. Borchers[1, 2, 3]; *[1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund, Germany; [2]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [3]Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; [4]Center for Proteomics and Metabolomics, Leiden University, Netherlands; [5]Institute for Biochemistry and Molecular Biology, Freiburg, Germany*

MP 052 **Drug Induced Protein Conformational and Interaction Dynamics by Quantitative Cross-linking Mass Spectrometry**; Juan D Chavez[1]; Devin K Schweppe[1]; Xuefei Zhong[1]; Jimmy K Eng[1]; James E Bruce[1]; *[1]University of Washington, Seattle, WA*

MP 053 **Circularization of Calmodulin by Disulfide Bond: Structural Characterization by LC-MS/MS and Effects on Protein Dynamics by Isothermo Titration Calorimetry**; You-Jun Fu[1]; Priya Katyal[1]; *[1]University of Connecticut, Storrs, CT*

MP 054 **Application of Fast Photochemical Oxidation of Proteins for *in vivo* Modification in Caenorhabditis elegans**; Lisa Jones[1]; Jessica A Espino[1]; *[1]University of Maryland, Baltimore, MD*

MP 055 **Dynamics of the Pre-amyloid Structural Change of β-2-microglobulin Studied by Covalent Labeling and Mass Spectrometry**; Blaise G Arden[1]; Nicholas B Borotto[1]; Brittney Burant[1]; Richard W Vachet[1]; *[1]University of Massachusetts-Amherst, Amherst, MA*

MP 056 **Protein Networks in Synaptic Vesicles Reveal Heterogeneous and Macromolecular Complexes that Mediate Signal Transduction in neuRons**; Sabine Wittig[1]; Carla Schmidt[1]; *[1]HALOmem, University of Halle, Halle / Saale*

MP 057 **Topographical Characterization of COSMC Using Hydroxyl Radical Protein Footprinting by Fast Photochemical Oxidation of Proteins**; Niloofar Abolhasani Khaje[1]; Pradeep Kumar Prabhakar[2]; Kelley W Moremen[2]; Joshua S. Sharp[1]; *[1]Department of Biomolecular Sciences, University of Mississippi, University, MS; [2]Complex Carbohydrate Research Center, University of Georgia, Athens, GA*

MP 058 **Starfish Relaxin-Type Dimeric Peptide Cross-Linked by Disulphide Bridgesanalysed by High Collision Energy (HCD) Fragmentation and Stavrox Software**; Cleidiane Zampronio[1]; Ming Lin[2]; Masatoshi Mita[3]; Michaela Egertová[2]; Alexandra M Jones[1]; Maurice R Elphick[2]; *[1]University of Warwick, Coventry, UK; [2]Queen Mary University of London, London, UK; [3]Tokyo Gakugei Univeristy, Tokyo, Japan*

MP 059 **Revealing Tertiary Structural Interactions of the Cellular Prion Protein through Chemical Cross-linking and Mass Spectrometry**; Deborah R. Leon[1]; Alex J. McDonald[1]; Christian F. Heckendorf[1]; Mark E. McComb[1]; Philip C. Andrews[2]; David A. Harris[1]; Catherine E. Costello[1]; *[1]Boston University School of Medicine, Boston, MA; [2]University of Michigan, Ann Arbor, MI*

MP 060 **Transcription factor-DNA Interaction Studied by Structural Mass Spectrometry**; Lukas Slavata[1, 2]; Michal Rosulek[1, 2]; Daniel Kavan[1, 2]; Alan Kadek[1, 2]; Petr Man[1, 2]; Petr Novak[1, 2]; *[1]BIOCEV - Institute of Microbiology of the CAS, v.v.i., Vestec, Czech Republic; [2]Faculty of Science, Charles University, Prague, Czech Republic*

MP 061 **Application of MS2-PD-MS3 Workflow for Large-Scale Identification of Cross-Linked Peptides**; Ievgen Motorykin[1]; Kumar Yugandhar[2]; Jin Liang[2]; Elizabeth T. Anderson[1]; Robert W. Sherwood[1]; Haiyuan Yu[2]; Sheng Zhang[1]; *[1]Mass Spectrometry and Proteomics Facility, Institute of Biotechnology, Cornell University, Ithaca, NY; [2]Weill Institute for Cell and Molecular Biology, Department of Biological Statistics and Computational Biology, Cornell University, Ithaca, NY*

MP 062 **Development of a Statistic-Based Potential for Chemical Cross-Linking/Mass Spectrometry Derived Constraints for Protein Tertiary Structure Determination**; Allan Jhonathan Ramos Ferrari[1]; Leandro Martínez[1]; Fabio Cesar Gozzo[1]; *[1]University of Campinas, Campinas, SP*

MP 063 **X-Ray Hydroxyl Radical Protein Footprinting of Intact, Functional Mitochondria** ; Awuri Asuru[1]; Jen Bohon[2, 3]; Janna Kieslar[1, 3]; Mark R. Chance[1, 2, 3]; *[1]Center for Proteomics and Bioinformatics, Case Western Reserve University, Cleveland, OH; [2]Center for Synchrotron Biosciences, Case Western Reserve University, Cleveland, OH; [3]Department of Nutrition, Case Western Reserve University, Cleveland, OH*

MP 064 **Characterizing a Plant Receptor Kinase's Three Dimensional Structure using Bottom Up Mass Spectrometry-Based Protein Footprinting**; Pei Liu[1]; Benjamin B. Minkoff[1]; Miyoshi Haruta[1]; Michael R. Sussman[1]; *[1]Department of Biochemistry and Biotechnology Center, University of Wisconsin, Madison, WI*

MP 065 **Dimethyl Labeling Coupled with Mass Spectrometry for Topographical Characterization of Primary Amines on Monoclonal Antibodies**; Sin-Yi Jhan[1]; Li-Juan Huang[1]; Shu-Hui Chen[1]; *[1]National Cheng Kung University, Tainan, Taiwan*

MP 066 **Application of MS3 Experiments to Confidently Identify Cross-linked Peptides**; Bingqing Zhao[1]; James P. Reilly[2]; *[1]IU, Bloomington, Indiana; [2]Indiana University, Bloomington, IN*

MP 067 **Interpretation of Anomalously Long Crosslinks in Ribosome Crosslinking**; Santosh A Misal[1]; James P. Reilly[2]; *[1]Indiana University Bloomington, Bloomington, IN; [2]Indiana University Bloomington, Bloomington, IN*

MP 068 **Defining the Structural Dynamics of Cullin-RING Ligase Complexes Using a Novel Multiplexed Quantitative Cross-linking Mass Spectrometry Strategy**; Clinton Yu[1]; Haibin Mao[2]; Alexander Huszaugh[1]; Rosa Viner[3]; Eric Novitsky[1]; Scott Rychnovsky[4]; Lan Huang[4]; *[1]University of California, Irvine, Irvine, CA; [2]University of Washington, Seattle, WA; [3]ThermoFisher, San Jose, CA; [4]University of California, Irvine, Irvine, CA*

MP 069 **Crosslinking Mass Spectrometry (XL-MS) Probes Changes in Protein Domain Structures and Distinguishes Rigid from Flexible Domains**; Lolita Piersimoni[1]; Manolo D Plasencia[1]; Hollis D Showalter[2]; Philip C Andrews[1, 3, 4]; *[1]Department of Biological Chemistry, University of Michigan, Ann Arbor, MI; [2]Department of Medicinal Chemistry, University of Michigan, Ann Arbor, MI; [3]Department of Chemistry, University of Michigan, Ann Arbor, MI; [4]Department of Computational Medicine and Bioinformatics, University of Michigan, Ann Arbor, MI*

MP 070 **Sequencing the RNA Moiety of Peptide-Oligonucleotide Cross-Links by nanoLC-ESI-MS/MS**; Aleksandar Chernev[1, 2]; Kuan-Ting Pan[1]; Uwe Pleßmann[1]; Henning Urlaub[1, 2]; *[1]Max Planck Institute for Biophysical Chemistry, Goettingen; [2]University Medical Center, Goettingen, Germany*

MP 071 **A Software Pipeline for Identifying and Validating Chemical Crosslink Sites in Nonspecifically-Digested LC-MS/MS Samples**; Mark E. Adamo[1]; Scott A. Gerber[1]; Andrew V. Grassetti[1]; *[1]Dartmouth College, Lebanon, NH*

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MP 072 **Uromodulin Isolation and Its Glycosylation Analysis by nanoLC-MS/MS**; Haiying Li[1]; Stephen Kostel[1]; John Froehlich[1]; Richard S. Lee[1]; *[1]Boston Children's Hospital, Boston, MA*

MP 073 **Automated Characterization of Isomeric N-glycans using Liquid Chromatography Tandem Mass Spectrometry (LC-MS/MS)**; Rui Zhang[1]; Xue Dong[2]; Yehia Mechref[2]; Haixu Tang[1]; *[1]Indiana University Bloomington, Bloomington, IN; [2]Texas Tech University, Lubbock, TX*

MP 074 **Development of a Multi-Dimensional HPLC-MS Method For Heparin/Heparan Sulfate Oligosaccharide Analysis**; Hao Liu[1]; Morgan Stickney[2]; Jonathan I Amster[2]; Joshua S. Sharp[1]; *[1]Department of BioMolecular Sciences, The University of Mississippi, Oxford, MS; [2]Department of Chemistry, University of Georgia, Athens, GA*

MP 075 **N-glycosylation Analysis of mAbs by CESI-MS at the Glycopeptide and Released Glycan Levels**; Jenny Albanese[1]; Marton Szigeti[2]; Bryan Fonslow[3]; Andras Guttman[3]; Edna Betgovargez[3]; *[1]SCIEX, Redwood City, CA; [2]University of Debrecen, Debrecen, Hungary; [3]Sciex, Brea, CA*

MP 076 **Skyline™-based Quantitative N-glycomics Reveals Altered Expression of Paucimannosidic N-glycans of Mouse Brain Tissues upon Neuropathic Pain Induction**; Christopher Ashwood[1, 2]; Vicky Staikopoulos[3, 4]; Arun V Everest-Dass[1, 2]; Morten Thaysen-Andersen[2]; Mark R Hutchinson[3, 4]; Nicolle H Packer[1, 2]; *[1]ARC Centre of Excellence in Nanoscale Biophotonics, Macquarie University, Sydney, Australia; [2]Department of Chemistry and Biomolecular Sciences, Macquarie University, Sydney, Australia; [3]ARC Centre of Excellence in Nanoscale Biophotonics, The University of Adelaide, Adelaide, Australia; [4]School of Medicine, The University of Adelaide, Australia*

MP 077 **Mild Acid Dissociation toward Defined Oligosaccharide Groups (MADDOG): A Universal Method for Structural Characterization of Polysaccharides by Nano-HPLC-Chip/Q-TOF Mass Spectrometry**; Matthew J. Amicucci[1, 2]; Ace G. Galermo[2]; Guy Treves[2]; Carlito B. Lebrilla[2]; *[1]UC Davis Agricultural and Environmental Chemistry Graduate Group, Davis, CA; [2]UC Davis Department of Chemistry, Davis, CA*

MP 078 **Sequence Analysis of Proteoglycan Decorin and Other Large Chain Glycosaminoglycan MS2 Using Automated Analysis Software**; Jiana Duan[1]; Agyekum Isaac[1]; I. Jonathan Amster[1]; *[1]University of Georgia, Athens, GA*

MP 079 **A Method for Distinguishing Arm-Specific Sialylation of Unsaturated Multiple-Antennae N-linked Glycan Isomers using Exoglycosidase Digestion by HT-PGC LC-MS/MS**; Chein-Hung Chen[1]; Ya-Ping Lin[1]; Fang-Chi liu[1]; Chi-Lin Wu[1]; Jung-Lee Lin[1]; Chung-Hsuan Chen[1]; *[1]Academia Sinica, Taipei, Taiwan*

MP 080 **Comparison of InstantPC and Traditional N-Glycan Labeling Dyes**; John Yan[1]; Andres Guerrero[1]; Steven Mast[1]; Emily Dale[1]; Ted Haxo[1]; Aled Jones[1]; *[1]ProZyme, Hayward, CA*

MP 081 **Automated and Rapid Characterization of Low-Molecular-Weight Heparin Oligosaccharides Using TripleTOF 5600 Mass Spectrometer with SimGlycan Software**; Ningombam Sanjib Meitei[1, 2]; Rajesh Pujari[1]; Arun Apte[2]; Annu Uppal[3]; *[1]PREMIER Biosoft, Indore, India; [2]PREMIER Biosoft, Palo Alto, CA; [3]SCIEX, Gurgaon, India*

MP 082 **High Throughput Analysis of N-Glycans Released from Biosimilar Glycoproteins**; Zoltan Szabo[1]; Shanhua Lin[1]; Dietmar Reusch[2]; Aled Jones[3]; John Yan[3]; *[1]Thermo Fisher Scientific, Sunnyvale, CA; [2]Roche Diagnostics GmbH, Penzberg, Germany; [3]ProZyme, Hayward, CA*

MP 083 **LC-MS/MS Isomeric Profiling of Permethylated N-Glycans Derived from Serum Haptoglobin of Hepatocellular Carcinoma (HCC) and Cirrhotic Patients**; Yifan Huang[1]; Shiyue Zhou[1]; Jianhui Zhu[2]; David M. Lubman[2]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX; [2]University of Michigan, Ann Arbor, MI*

MP 084 **Isomeric Complexity of Glycosylation in MCF-7 and MDA-MB-231 Cell Lines Revealed by Detailed Analysis with Ion Trap Mass Spectrometry**; David Ashline[1, 2]; Hailong Zhang[2]; Vernon N. Reinhold[2]; *[1]Glycan Connections, Dover, NH; [2]University of New Hampshire, Durham, NH*

MP 085 **16-plex/32-plex LC-MS Analysis of Isotopically Permethylated N-glycans Derived from Biological Samples**; Xue Dong[1]; Wenjing Peng[1]; Yifan Huang[1]; Seth D Williamson[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

MP 086 **Microscale Chemical Release of O-linked Oligosaccharides by RAIDR**; Lucas Veillon[1]; Ahmed Hussein[1, 2]; Byeong G Cho[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX; [2]Alexandria University, Alexandria, Egypt*

MP 087 **Structure Analysis of Glycosaminoglycan Intermediate Oligosaccharides Elongated on β-xylosides**; Yuya Otsuka[1, 2]; Toshinori Sato[2]; *[1]Seikagaku Corporation, Higashiyamato-shi, Japan; [2]Department of Biosciences and Informatics, Keio University, Yokohama, Japan*

MP 088 **Effectiveness of N-linked Glycan Release: A Quantitative Comparison of Chemical Release versus PNGase F Release Protocols**; David Fischler[1]; Ron Orlando[1]; *[1]Complex Carbohydrate Research Center, University of Georgia, Athens, GA*

MP 089 **Mass Spectrometry-Based Quantitative Analysis for Decoding Site-Specific Alteration of Sialo-glycoproteome in EGFR-subtypes of Non-Small Cell Lung Cancers**; Yi-Ju Chen[1]; Yu-Hsien Lin[2]; Ta-Chi Yen[1]; Kay-Hooi Khoo[3]; Yu-Ju Chen[1]; *[1]Institute of Chemistry, Academia Sinica, Taipei City, Taiwan; [2]Institute of Chemistry, Academia Sinica,, Taipei City, Taiwan; [3]Institute of Biological Chemistry, Taipei City, Taiwan*

MP 090 **Purification of Permethylated N-glycans by using Carbon Nanoparticles: Enhancing Sensitivity and Mass Accuracy**; Jieqiang Zhong[1]; Alireza Banazadeh[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

MP 091 **A Universal Approach to linkage-Specific Derivatization for Sialic Acids on Glycopeptides**; Takashi Nishikaze[1]; Sadanori Sekiya[1]; Shinichi Iwamoto[1]; Koichi Tanaka[1]; *[1]Shimadzu Corporation, Kyoto, Japan*

MP 092 **Exploring the Species-specific Glyco-biosynthesis via Nano-LC/MS and LC/MS/MS for the Development of Humanized Mouse Model**; Dan Bi Park[1, 2]; Sumin Kim[2, 3]; Jeong Gu Kang[4]; Yong-Sam Kim[4]; Jong Shin Yoo[5]; Jeong-Heon Ko[4]; Hyun Joo An[1, 2]; *[1]Asia Glycomics Reference Site, Chungnam National University, South Korea; [2]Graduate School of Analytical Science and Technology, Daejeon, South Korea; [3]Asia Glycomics Reference Site, Daejeon, South Korea; [4]Korea Institute of Bioscience and Biotechnology, Daejeon, South Korea; [5]Korea Basic Science Institute, Cheongju , Chungbuk*

MP 093 **Isomeric Separation and identification of Standard Glycans and Glycans in Model Glycoproteins by PGC-LC-MS/MS at High Temperature**; Aiying Yu[1]; Yifan Huang[2]; Shiyue Zhou[2]; Xue Dong[2]; Yehia Mechref[2]; *[1]Texas Tech University, Lubbock, TX; [2]Texas Tech University, Lubbock, TX*

MP 094 **Carbon Nanoparticles and Graphene Nanosheets as MALDI Matrices in Glycemics: A New Approach to Improve Glycan Profiling in Biological Samples**; Alireza Banazadeh[1]; Wenjing Peng[1]; Lucas Veillon[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, Texas*

MP 095 **Fixed Ligand Kinetic Method to Determine the Preservation of Stoichiometry in the Solvolysis of Carbohydrates**; Zachary Wooke[1]; Nicola L. B. Pohl[1]; *[1]Indiana University, Bloomington, IN*

MP 096 **Detailed Structural Analyses of O-glycan Alditols by High Performance Anion Exchange Chromatography (HPAE) Coupled to Mass Spectrometry**; Zoltan Szabo[1]; Niclas G Karlsson[2]; Dietmar Reusch[3]; Jim Thayer[4]; Yury Agroskin[4]; Rosa Viner[5]; Gina Tan[5]; Andreas F. Huhmer[5]; Christopher Pohl[4]; *[1]Thermo Fisher Scientific, Sunnyvale, CA; [2]University of Gothenburg, Gothenburg, Sweden; [3]Roche Diagnostics GmbH, Penzberg; [4]Thermo Fisher Scientific, Sunnyvale, CA; [5]Thermo Fisher Scientific, San Jose, CA*

MP 097 **The Outermost Surface N-glycomic Analysis of Breast Cancer Cell Lines using PNGase F Digestion on living Cells**; Wenjing Peng[1]; Akhila Reddy[1]; Jingfu Zhao[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

MP 098 **Isomeric N-glycan Analysis of Breast Cancer Cell Lines using Porous Graphitic Carbon (PGC) Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS)**; Mona Goli[1]; Wenjing Peng[1]; Xue Dong[1]; Shiyue Zhou[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

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MP 099 **Quantitation of Putative Colorectal Cancer Biomarker Candidates in Serum Extracellular Vesicles by Targeted Proteomics**; Takeshi Tomonaga[1]; Takashi Shiromizu[1]; Jun Adachi[1]; *[1]Laboratory of Proteome Research, National Institutes of Biomedical Innovation, Health and Nutrition, Ibaraki, Japan*

MP 100 **Modern Orbitrap Based Mass Spectrometers Detect an Unexpected Multitude of Proteoforms in (Human) Secretory Fluids: PROTEOFORMICS of the Human Tear**; Peter D. Verhaert[1]; Peter P. Raus[2]; Martijn W. Pinkse[1]; PAUL THOMAS[3]; Neil L Kelleher[3]; *[1]Delft University of Technology, DELFT, Europe; [2]Miró Center, Geel, Belgium; [3]Northwestern University, Evanston, IL*

MP 101 **iKnife Rapid Evaporative Ionisation Mass Spectrometry (REIMS) Technology In Head and Neck Surgery. A *ex vivo* Feasibility Study**; Jagtar Dhanda[1]; Andrew Schache[2]; Max Robinson[3]; Zsolt Bodai[4]; Emma L. White[4]; Burak Temelkuran[4]; Yang Guang-Zhong[4]; Zoltan Takats[4]; *[1]Queen Victoria Hospital, East Grinstead, UK; [2]University of Liverpool, Liverpool, Merseyside; [3]Universit of Newcastle, Newcastle upon Tyne, UK; [4]Imperial College London, London, UK*

MP 102 **Investigating Paper Properties for Ion Suppression and Recovery in Paper Spray Mass Spectrometry**; Brandon Bills[1]; Jeffrey Kinkade[1]; Nicholas Manicke[1]; *[1]IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN*

MP 103 **Quantitative Proteomic Analysis of MGMT May Predict Response of Colorectal Cancer Patients to Treatment with Temozolomide**; Yuan Tian[1]; Sarit Schwartz[1]; Wei-li Liao[1]; Fabiola Cecchi[1]; Filippo Pietrantonio[2]; Todd Hembrough[1]; *[1]Nantomics, Rockville, MD; [2]Fondazione IRCCS Istituto Nazionale dei Tumori, Milan, Italy*

MP 104 **Breath Analysis with Thermal Desorption-Field Asymmetric Ion Mobility Spectrometry-Mass Spectrometry: A Rapid and Non-Invasive Means of Screening for Pulmonary-Related Diseases**; Alasdair Edge[1]; Lauren Brown[1]; Kayleigh Arthur[1]; Robert Smith[1]; *[1]Owlstone Medical Ltd., Cambridge, UK*

MP 105 **Background Proteins in hCG Formulations of Different Manufacturers**; Goran Mitulovic[1]; Tanja Panić-Janković[1]; *[1]Medical University of Vienna, KIMCL, Vienna, Austria*

MP 106 **Requirements for Successful Development of MS-based Protein Assays that Target Unmet Clinical Needs**; Yuri E. M. van der Burgt[1]; L. Renee Ruhaak[1]; Nico P. M. Smit[1]; Fred P. H. T. M. Romijn[1]; Arnoud van der Laarse[1]; Wilma E. Mesker[1]; Rob A. E. M. Tollenaar[1]; Magnus Palmblad[1]; Manfred Wuhrer[1]; Christa M. Cobbaert[1]; *[1]Leiden University Medical Center, Leiden, Netherlands*

MP 107 **Role of RNase L in Kideny**; Norah Alghamdi[1]; Danting Liu[1]; Ruhan Wei[1]; Aimin Zhou[1]; *[1]Cleveland State University, Department of Chemistry, Cleveland, OH*

MP 108 **LC-MS-MS Quantitative Analysis of Retinoids and Metabolites in Serum for Research Use**; Rory M Doyle[1]; Joshua Kilne[1]; *[1]Thermo Fisher Scientific, Somerset, NJ*

MP 109 **A New Tool for the Automated Sample Preparation of Whole Blood Samples by LC-MS using a Commercial Autosampler**; Guenter Boehm[1]; Christian Berchtold[2]; Reto Bolliger[1]; Renzo Picenoni[1]; Thomas Preiswerk[1]; Goetz Schlotterbeck[2]; *[1]CTC Analytics AG, Zwingen, BL; [2]Fachhochschule Nordwestschweiz, Muttenz, Switzerland*

MP 110 **Routine 50uL Serum/Plasma Analysis of Hepcidin-25, Hepcidin-20, Hepcidin-22 and Hepcidin-24 using LC/MS/MS: Diurnal Study**; Benjamin Hunter[1]; Robert Trengove[1]; Joel Gummer[1]; *[1]Murdoch University, Murdoch , WA*

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Germany; [4]Dept. of Surgery, Maastricht University Medical Centre, Maastricht, Netherlands

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MP 144 **Development of a Magnetic Microbead Affinity Selection Screening (MagMASS) UHPLC-MS Assay for the Progesterone Receptor**; Daniel Nosal[1]; Michael D Rush[1]; Tristesse Burton[1]; Richard van Breemen[1]; *[1]University of Illinois at Chicago College of Pharmacy, Chicago, IL*

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MP 147 **An Open Port Sampling Interface for High-Throughput SPME-MS/MS analysis of *in vitro*ADME Samples**; John Janiszewski[1]; Brendon Kapinos[2]; Sara Smith[3]; Craig Aurand[3]; Chang Liu[4]; Tom Covey[4]; German Augusto Gomez-Rios[5]; *[1]Pfizer Inc., Groton, CT; [2]Pfizer Inc., Groton, CT; [3]MilliporeSigma, Bellefonte, PA; [4]SCIEX, Concord, ON, Canada; [5]University of Waterloo, Waterloo, Ontario*

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MP 166 **Molecular Characterization of Naphthenic Acids Extracted from a Heavy Crude Oil using MALDI FTICR Mass Spectrometry**; Jeferson A. Valencia-Dávila[1]; Matthias Witt[2]; Cristian Blanco-Tirado[1]; Marianny Y. Combariza[1]; *[1]Universidad Industrial de Santander, Bucaramanga, Colombia; [2]Bruker Daltonik GmbH, Bremen, Germany*

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MP 168 **Application of On-line Liquid Chromatography Coupled to Ultra-High Resolution 21 T FT-ICR Mass Spectrometry for Petroleum Analysis**; Donald F. Smith[1]; Steven M. Rowland[1, 2]; Greg T. Blakney[1]; Yuri E. Corilo[1, 2]; Christopher L. Hendrickson[1, 2, 3]; Ryan P. Rodgers[1, 2, 3]; *[1]National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; [2]Future Fuels Institute, Florida State University, Tallahassee, FL; [3]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL*

MP 169 **Estimation of Confidence in Assigning True Molecular Formulae of Complex Mixtures**; Yuri E. Corilo[1, 2]; Melaine C. De Oliveira[3]; Donald F. Smith[4]; Ryan P. Rodgers[2, 4, 5]; Christopher L. Hendrickson[2, 4, 5]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]Future Fuels Institute, Florida State University, Tallahassee, Florida; [3]Department of Statistics, Florida State University, Tallahassee, FL; [4]National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; [5]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL*

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MP 173 **Comparison of Atmospheric Pressure Chemical Ionization and Field Ionization Mass Spectrometry for the Analysis of Large Saturated Hydrocarbons**; Yuyang Zhang[1]; Chunfen Jin[1]; Jyrki Viidanoja[2]; Jeremy Manheim[1]; Mingzhe Li[1]; Hilkka Kenttamaa[1]; *[1]Purdue University-Department of Chemistry, West Lafayette, IN; [2]Neste Corporation, Finland*

MP 174 **Differentiation of Isomeric Hydrocarbon Ions Containing Five- and Six-Membered Naphthene Rings by using Energy-Resolved Medium Energy Collision-Activated Dissociation (MCAD)**; Mark Romanczyk[1]; Jyrki Viidanoja[2]; Hilkka Kenttamaa[1]; *[1]Purdue University-Department of Chemistry, West Lafayette, IN; [2]Thermo Fisher Scientific, Vantaa, Finland*

MP 175 **Structural Determination of Polycyclic Aromatic Hydrocarbons by Ion Mobility Mass Spectrometry**; Priscila M. Lalli[1, 2]; Yuri E Corilo[2, 3]; Martha L. Chacón-Patiño[3]; RYAN P. RODGERS[2, 3, 4]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]Future Fuels Institute, Florida State University, Tallahassee, FL; [3]National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; [4]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL*

MP 176 **Direct Infusion APCI MS Analysis of Mixtures of Large Saturated Hydrocarbons by Using Different Hydrocarbon Solvents**; Jeremy Manheim[1]; Yuyang Zhang[1]; Chunfen Jin[1]; Jyrki Viidanoja[2]; Hilkka Kenttamaa[1]; *[1]Purdue University-Department of Chemistry, West Lafayette, IN; [2]Neste Corporation, Finland*

MP 177 **Acceleration of Field-Activated TiO2-catalyzed Oil Degradation in Microdroplets**; Yin-Hung Lai[1]; Zhenpeng Zhou[1]; Chanbasha Basheer[2]; Richard N Zare[1]; *[1]Stanford University, Stanford, CA; [2]Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia*

MP 178 **FT-ICR-MS Data Provide Structural Features of Heavy Crude Oil Components**; Cristian Blanco-Combariza[1]; Marianny Y Combariza[1]; Cristian Blanco-Tirado[1]; *[1]Universidad Industrial de Santander, Bucaramanga, Colombia*

MP 179 **Portable H2 Sensor**; Takashi Nohmi; *HysafeNohmi, Setagaya-Ku, Japan*

MP 180 **Prediction of the SARA Analysis of Colombian Crude Oils Using APPI(+)-FTICR MS Coupled to PLS with GA Variable Selection**; Enrique Mejia-Ospino[1]; Diana Catalina Palacio[1]; Jorge A. Orrego-Ruiz[2]; Jader E. Guerrero[1]; Rafael Cabanzo[1]; *[1]Universidad Industrial de Santander, Bucaramanga, SDER; [2]Instituto Colombiano de Petróleos (ICP), Piedecuesta, Colombia*

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MP 183 **Detection of Harmful Carbonyl Compounds in E-Cigarette Liquids via *in-situ* Derivatization Nano-Electrospray Ionization Mass Spectrometry**; Tavleen K. Kochar[1]; Gary L. Glish[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC*

MP 184 **Investigation of Extracted and Leached Analytes from Packaging Materials with GC-MS and High Resolution MS**; Elizabeth Humston-Fulmer[1]; Joe Binkley[1]; *[1]LECO Corporation, Saint Joseph, MI*

MP 185 **Direct Analysis of Glyphosate in wine with No Sample Preparation using an LC-MS/MS System with a Stay Clean Source** ; Sharanya Reddy[1]; Matteo Meglioli[2]; Frank Kero[1]; *[1]PerkinElmer, Shelton , CT; [2]Mosti Mondiale Inc, Québec, QC, Canada*

MP 186 **Ion Mobility for Food Safety: Extensive Comparison of Ion Mobility Mass Spectrometry Instruments**; Wilco F. Duvivier[1]; Marco H. Blokland[1]; Michel W.F. Nielen[1, 2]; *[1]RIKILT Wageningen University & Research, Wageningen, Netherlands; [2]Laboratory of Organic Chemistry, Wageningen, Netherlands*

MP 187 **A Multi-Laboratory Comparison of MS Platforms for the Targeted Analysis of Peanut in Food**; Victoria Lee[1]; Rebekah L Sayers[1]; Ivona Baricevic-Jones[1]; Carol-Ann Costello[1]; Sabine Baumgartner[2]; Christine H Parker[3]; Gavin O'Connor[4]; Philip Johnson[5]; E. N. C Mills[1]; *[1]University of Manchester, Manchester, UK; [2]University of Natural Resources and Life Sciences - BOKU, Vienna, Austria; [3]FDA Center for Food Safety, College Park, MD; [4]JRC IRMM, Geel, Belgium; [5]University of Nebraska, Lincoln, NE*

MP 188 **Determination of multiple pesticide residue in Green Chilli by GC-MS/MS using Modified QuEChERS as an Extraction Method**; Sanket Chiplunkar[1]; Dheeraj Handique[1]; Ankush Bhone[1]; Prashant Hase[1]; Durvesh Sawant[1]; Nitish Suryawanshi[1]; Ajit Datar[1]; Jitendra Kelkar[1]; Pratap Rasam[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

MP 189 **Highly Sensitive and Rapid Analysis of Synthetic dyes in Sea Food by LC/MS/MS**; Shailesh Damale[1]; Anant Lohar[1]; Shailendra Rane[1]; Purushottam Sutar[1]; Ashutosh Shelar[1]; Deepti Bhandarkar[1]; Rashi Kochhar[1]; Jitendra Kelkar[1]; Pratap Rasam[1]; Ajit Datar[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

MP 190 **Determination of Polycyclic Aromatic Hydrocarbons in a Candidate Yerba Mate Standard Reference Material by GC-MS**; Jacolin A. Murray[1]; Michele M. Schantz[1]; Laura J. Wood[1]; Melissa M. Phillips[1]; Stephen A. Wise[1, 2]; *[1]National Institute of Standards and Technology, Gaithersburg, MD; [2]National Institutes of Health, Bethesda, MD*

MP 191 **LC-MS/MS and DART-HRMS Screening of Beverages for Sweeteners**; Luke K Ackerman[1]; Nicole Shyong[1]; *[1]FDA Center for Food Safety, College Park, MD*

MP 192 **A Novel Fast and Simple Quantification Method for Vitamins, Complements and contaminants in Milk Infant Formulas by LC-MS/MS**; Aurore Jaffuel[1]; Thierry Legoupil[1]; Alban Huteau[1]; *[1]Shimadzu France, Paris, France*

MP 193 **Improving Gas Chromatograph-Mass Spectrometer System Longevity for Multi-Residue Pesticide Methods in Matrix Through Inert Microfluidic Retention Gap Technology**; Rebecca Veeneman[1]; Matthew Giardina[1]; *[1]Agilent Technologies, Wilmington, Delaware*

MP 194 **Sample Profiler: A Cloud Based Application for Confirming Food Authenticity**; Srividya Kailasam[1]; Ralf Tautenhahn[2]; Tim J. Stratton[2]; *[1]Thermofisher Scientific, Bangalore, India; [2]ThermoFisher, San Jose, CA*

MP 195 **Application of SFC-MS/MS for the Quantification of Highly Polar Pesticides in a Range of Food Samples**; David Baker[1]; Chris Titman[1]; Jonathan Horner[2]; Neil Loftus[1]; *[1]Shimadzu, Manchester, UK; [2]Scientific Analysis Laboratories, Cambridge, UK*

MP 196 **Screening of Pesticides and other contaminants in Food Matrices using a Novel High Resolution GC/Q-TOF with Low-Energy Capable EI Source**; Kai Chen[1]; Jennifer Sanderson[1]; *[1]Agilent Technologies, Santa Clara, CA*

MP 197 **Using Pressurized Liquid Extraction for the Extraction and Analysis of Pesticides in Cannabis Samples**; Philip M Germansderfer[1]; Hamid R Shirkhan[1]; *[1]Fluid Management Systems, Watertown, MA*

MP 198 **Direct Analysis of glyphosate and Similar Polar Pesticides in Various Food Matrices**; Dimple Shah[1]; Euan Ross[2]; Benjamin Wuyts[2]; Eimear McCall[2]; Gareth Cleland[1]; Kenneth Rosnack[1]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK*

MP 199 **Automated Extraction and Clean Up of POPs Using a Green Low Solvent System**; Hamid R Shrikhan[1]; Waleed Hassan[1]; *[1]Fluid Management Systems, Watertown, MA*

MP 200 **Multiresidue Pesticide Analysis in Fruit and Vegetable Commodities Using Both UPLC and APGC on a Single Mass Spectrometer Platform**; Kari Organtini[1]; Eimear McCall[2]; Gareth Cleland[1]; Kenneth Rosnack[1]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK*

MP 201 **Advances in Ion Mobility Mass Spectrometry to Further Characterize Contaminants in Food**; Lauren Mullin[1, 2]; Gareth Cleland[1]; Andrew Baker[3]; Mike McCullagh[4]; Sara Stead[4]; Kenneth Rosnack[1]; Joe Romano[1]; *[1]Waters Corporation, Milford, MA; [2]Örebro University, Örebro, Sweden; [3]Waters Corporation, Pleasanton, CA; [4]Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK*

MP 202 **Development of a Comprehensive Multiplex Allergen Detection MRM Method for Standardized Food Testing**; Derek Croote[1]; Ido Braslavsky[2]; Karolina M Krasinska[3]; Stephen R Quake[1]; *[1]Stanford University, Stanford, CA; [2]Hebrew University, Jerusalem, Israel; [3]Stanford University Mass spectrometry, Stanford, CA*

MP 203 **Target Peptide Identification for the Mass Spectrometric Detection of Soy Proteins in Food Matrices**; Shimin Chen[1]; Charles Yang[2]; Melanie Downs[1]; *[1]Food Allergy Research and Resource Program, Department of Food Science and Technology, University of Nebraska-Lincoln, Lincoln, NE; [2]Thermo Fisher Scientific, San Jose, CA*

MP 204 **Analysis of Polychlorinated Biphenyls in Coffee using Automated Extraction and Reduced Solvent Volume Clean Up**; Thomas G Hall[1]; Alexander Sharapov[1]; *[1]Fluid Management Systems, Watertown, MA*

MP 205 **Fully Automated Derivatization -Quantification of Glyphosate and AMPA in Beer using a Standard UHPLC-MS/MS System**; Julia Sander[1]; Anja Grüning[1]; Robert Ludwig[1]; Philipp Jochems[1]; *[1]Shimadzu Europa GmbH, Duisburg, Germany*

MP 206 **Analysis of Mycotoxins in Cereal and Corn without Derivatization via LC-MS/MS with Time-Managed MRMs**; Wilhad Reuter[1]; Avinash Dalmia[1]; *[1]PerkinElmer Inc, Shelton, CT*

MP 207 **A Data-dependent Workflow for Selection of Peptide Targets for Robust Detection of allergens in Difficult Food Matrices**; Justin T Marsh[1]; Charles Yang[2]; Philip Johnson[1]; *[1]University of Nebraska, Lincoln, NE; [2]Thermo Fisher Scientific, San Jose, CA*

MP 208 **Fast and Extended Analysis of 213 FDA Regulated Pesticides in Organic and Non-organic Grapes by LC-MS/MS using Time-Managed-MRM**; Joshua Ye[1]; Feng Qin[1]; Shixin Sun[1]; Avinash Dalmia[2]; Wilhad Reuter[2]; Sergey Rakov[2]; Jamie Foss[3]; Frank Kero[3]; *[1]PerkinElmer LAS Canada Inc, Woodbridge, ON, Canada; [2]PerkinElmer Inc, Shelton, CT; [3]PerkinElmer, Downers Grove, IL*

MP 209 **Analytical Confirmation of Sildenafil Analogues Adulterated in Dietary Supplements**; Nam Sook Kim[1]; Ji Hyun Lee[1]; Kyu Yeon Kim[1]; Han Na Park[1]; Hyoung-Joon Park[1]; Taeik Hwang[1]; Seok Heo[1]; Jeong-Hwa Cho[1]; Jun-hyoung Kim[1]; Dong Woo Shin[1]; Seongsoo Park[1]; Sung-Kwan Park[1]; Sun Young Baek[1]; *[1]Ministry of Food and Drug Safety, Cheongju-si, Chungcheongbuk-do*

MP 210 **Released Volatiles Analysis of Flavor Capsules in Cigarette Filter under Simulated Working Conditions by Headspace-GC×GC-MS**; Xiangyu Li[1]; Hongfei Zhang[1]; Xingyi Jiang[1]; Yanbo Luo[1]; Fengpeng Zhu[1]; Shaodong Hu[1]; Yongqiang Pang[1]; *[1]China National Tobacco Quality Supervision & Test Centre, Zhengzhou, China*

MP 211 **Fast and Robust Multiresidue Analysis of Highly Polar Pesticides by Ion Chromatography Coupled to High Resolution Mass Spectrometry**; Łukasz Rajski[1];

Francisco José Díaz-Galiano[1]; Víctor Cutillas[1]; Amadeo R. Fernández-Alba[1]; *[1]European Union Reference Laboratory for Pesticide Residues in Fruit & Vegetables, Almería, Spain*

MP 212 **Infant Exposure to Arsenic and Lead From Rice Cereal and Bottled Water**; Marc E. Engel[1]; Donald M Axelrad[2]; *[1]FDACS, Tallahassee , FL; [2]Florida A&M University College of Pharmacy and Pharmaceutical Sciences Institute of Public Health, Tallahassee, FL*

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MP 213 **Multiplexing Hard and soft Electron Ionisation for Improved Speciation of Cannabinoids**; Chris Hall[1]; Natasha Spadafora[1]; Laura McGregor[1]; Matthew Edwards[2]; Pete Grosshans[1]; Nick Bukowski[1]; *[1]Markes International, Llantrisant , Cardiff; [2]SepSolve Analytical, Peterborough, UK*

MP 214 **Screening of Drugs of Abuse and Pesticides in Liver following Homogenization and Supported Liquid Extraction (SLE) prior to GC/MS Analysis**; Rhys Jones[1]; Katie-Jo Teehan[1]; Lee Williams[1]; Geoff Davies[1]; Helen Lodder[1]; Adam Senior[1]; Alan Edgington[1]; Steve Jordan[1]; Claire Desbrow[1]; Paul Roberts[1]; *[1]Biotage GB Limited, Cardiff*

MP 215 **Direct Detection of Security Relevant Substances on Surfaces via Ambient Pressure Laser Desorption Mass Spectrometry**; René Reiss[1]; Sven Ehlert[1, 2]; Ralf Zimmermann[1, 3]; *[1]University of Rostock, Department of Analytical Chemistry, Rostock, Germany; [2]Photonion GmbH, Schwerin, Germany; [3]Joint Mass Spectrometry Centre, Comprehensive Molecular Analytics, Helmholtz Zentrum München, München, Germany*

MP 216 **Chemical Imaging of Cyanoacrylate Fumed Fingerprints Using MALDI-Orbitrap**; Kelly O'Neill[1]; Paige Hinners[1]; Young-Jin Lee[1]; *[1]Iowa State University, Ames, IA*

MP 217 **Rapid Screening and Determination of New Psychoactive Substances by Direct Analysis in Real Time Mass Spectrometry and LC/QTOFMS**; Honggang Nie[1]; Xianjiang Li[1]; Zhendong Hua[2]; Wei Pan[1]; Xiaofang Fu[1]; *[1]Peking University, Beijing, Beijing; [2]National Narcotics Laboratory, Beijing, China*

MP 218 **Chemical Identification in Latent Fingerprints for Lifestyle Determination**; Paige Hinners[1]; Kelly O'Neill[1]; Young-Jin Lee[1]; *[1]Iowa State University, Ames, IA*

MP 219 **An LC-QTOF-MS Assay for Post-Mortem Drug Screening in Dental Hard Tissue Samples**; Laura M. Huppertz[1]; Miriam Klima[1]; Miriam C. Kuales[2]; Markus J. Altenburger[2]; Volker Auwärter[1]; Merja A. Neukamm[1]; *[1]Institute of Forensic Medicine, Forensic Toxicology, Medical Center - University of Freiburg, Freiburg, Germany; [2]Center for Dental Medicine, Department of Operative Dentistry and Periodontology, Medical Center - University of Freiburg, Freiburg, Germany*

MP 220 **Paper Cone Spray Ionization Sources Featuring Integrated Extraction and Filtration for On-Site Forensic Applications**; William L. Fatigante[1]; Zachary E. Lawton[1]; Alessandra M. Bruno[1]; Shahnaz Mukta[1]; Michael C. Gizzi[1]; Christopher C. Mulligan[1]; *[1]Illinois State University, Normal, IL*

MP 221 **Development of Laser Ablation Direct Analysis in Real Time Imaging Mass Spectrometry (LADI-MS): Applications to Forensics Imaging**; Kristen Fowble[1]; Rabi A Musah[1]; *[1]University at Albany, Albany, NY*

MP 222 **Speciation of Antimony in Biological Samples by Liquid Chromatography-Inductively Coupled Plasma-Mass Spectrometry**; Yuko Kazui[1]; Yasuo Seto[1]; Shinichi Suzuki[1]; Yasuhiro Suzuki[1]; Ritsuko Sugita[1]; Hikoto Ohta[1]; Masaaki Kasamatsu[1]; Hajime Miyaguchi[1]; Takao Igawa[1]; *[1]National Research Institute of Police Science, Kashiwa*

MP 223 **Collection and Analysis of Drugs using Electrospun Nanofibers with Microfluidic Extraction and Tandem Mass Spectrometry**; Yufei Chen[1]; Pei Zhu[2]; Xiangwu Zhang[1]; Nelson Vinueza[2]; *[1]North Carolina State University, Raleigh, NC; [2]North Carolina State University, Raleigh, NC*

MP 224 **The Detection of Designer Drugs from Plasma via Paper Spray Mass Spectrometry**; Greta Jakstonyte Ren[1]; Nicholas Manicke[1]; *[1]IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN*

MP 225 **Separation and Identification of Organic Compounds in Gun Powders Using LC-MS Techniques**; Danielle Kirby[1]; Michael J. Van Stipdonk[1]; Stephanie J. Wetzel[1]; Logan Miller[1]; Kyle Brown[1]; *[1]Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA*

MP 226 **LC-MSMS Analysis of Hair Samples for the Detection of Prohibited Substances in Equine and Canine Sport**; Bob Gray[1]; Marjaana Viljanto[1]; Eleanor Menzies[1]; Stephanie Thompson[1]; Erin Crum[1, 2]; James Scarth[1]; *[1]LGC Ltd, Middlesex; [2]LGC Ltd US, lexington, KY*

MP 227 **Detection of Antifungal Drugs and Their Main Metabolites in Human Urine by LC-MS-based Techniques: Implications in Doping Analysis**; Monica Mazzarino[1]; Fabio Comunità[1]; Xavier de la Torre[1]; Francesco Botrè[1, 2]; *[1]Antidoping Laboratory of Rome, Rome, Italy; [2]Università degli studi di Roma "Sapienza", Rome, Italy*

MP 228 **Using Differential Mobility Spectrometry to Separate Chiral Compounds: Amphetamines**; J. Larry Campbell[1]; J.C. Yves Leblanc[2]; Chang Liu[2]; *[1]SCIEX, Concord, ON, Canada; [2]SCIEX, Concord, ON, Canada, ON, Canada*

MP 229 **Multivariate Data Interpretation of Direct Biomarkers of Ethanol Consumption for Forensic Purposes**; Marco Vincenti[1, 2]; Eugenio Alladio[1, 2]; Martyna Agnieszka[3]; Alberto Salomone[2]; Valentina Pirro[4]; Grzegorz Zadora[3, 5]; *[1]Dept. of Chemistry, Università di Torino, Torino, Italy; [2]Centro Regionale Antidoping e di Tossicologia "A. Bertinaria", Orbassano (Torino), Italy; [3]Department of Analytical Chemistry, The University of Silesia, Katowice, Poland; [4]Dept. of Chemistry, Purdue University, West Lafayette, IN; [5]Institute of Forensic Research, Krakow, Poland*

MP 230 **Compact Mass Spectrometer (CMS) Analysis of Uniformly 13C-labeled Amino Acids to Identify Authentic Therapeutic Drugs and Protect against Counterfeits**; Daniel Eikel[1]; Simon J Prosser[2]; Chris Beecher[3]; *[1]Advion Inc., Ithaca, NY; [2]Advion Inc., Ithaca, NY; [3]IROA Technologies, Bolton, MA*

MP 231 **Development of a Portable nLC-EI-MS**; Clyde Hale[1]; Mehdi Moini[2]; *[1]George Washington University , Washington, DC; [2]George Washington University, Washington, DC*

MP 232 **Comparison between DSA TOF-MS and DART TOF-MS for the Analysis of Writing Inks**; Nicholas L. Drury[1]; Mehdi Moini[2]; *[1]George Washington University , Washington, DC; [2]George Washington University, Washington, DC*

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MP 234 **Sonic Versus ESI Ionization for Noncovalent Interactions**; Abdil Ozdemir[1]; Mustafa Gulfen[1]; Jung-Lee Lin[2]; Chung-Hsuan Chen[2]; *[1]Sakarya University , Adapazari, Sakarya; [2]Academia Sinica, Taipei, Taiwan*

MP 235 **Opposite Polarity Electrical Charge on Electrosprayed Bacterial Spores: Implications for Electrospray Mechanism**; Jiuzhi Gao[1]; Ames Ettinger[1]; Richard A. Robison[1]; Daniel E. Austin[1]; *[1]Brigham Young University, Provo, UT*

MP 236 **Proteins Unfold During Supercharging Electrospray Ionization: Evidence from Ion Mobility-Mass Spectrometry Charge and Size Scaling Behavior**; Micah T. Donor[1]; Simon A. Ewing[1]; Muhammad A. Zenaidee[2]; William A. Donald[2]; James S. Prell[1]; *[1]University of Oregon, Eugene, OR; [2]University of New South Wales, Sydney, Australia*

MP 237 **Comparing the Effects of Additives on Protein Analysis by DESI and ESI**; Elahe Honarvar[1]; Andre R. Venter[1]; *[1]Western Michigan University, Kalamazoo, MI*

MP 238 **Understanding Electrospray Ionization Mechanisms of Biomolecules using In-Plume Laser-Induced Fluorescence**; Prince Tiwari[1]; Martin F. Czar[1]; Renato Zenobi[1]; *[1]ETH Zurich, Department of Chemistry and Applied Biosciences, Zurich, Switzerland*

MP 239 **Optimization of Electrospray Ionization Conditions for Enhanced Protonation of Small Peptides by Chromium(III)**; Juliette Joan Commodore[1]; Carolyn J Cassady[1]; *[1]The University of Alabama, Tuscaloosa, AL*

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MP 241 **Electron Transfer Dissociation and Collision-Induced Dissociation of Trivalent Metal-Adducted Oligosaccharides**; Ranelle Schaller-Duke[1]; Carolyn J Cassady[2]; *[1]The University of Alabama, Tuscaloosa, Al; [2]The University of Alabama, Tuscaloosa, AL*

MP 242 **Exploring Halide Anion Affinity of Cyclodextrins by Electrospray Ionization Mass Spectrometry and Molecular Modeling**; Chongsheng Xu[1]; Yanqiu Chu[1]; Chuan-Fan Ding[1]; *[1]Fudan University, Shanghai, Shanghai*

MP 243 **Using a Priori Intrinsic Size Parameters to Predict Ion Mobilities and Understand the Folding Patterns of Modified and Metalated Peptides**; Julia L. Kaszycki[1]; Matthew A. Baird[1]; Andrew P. Bowman[1]; Alexandre A. Shvartsburg[1]; *[1]Wichita State University, Wichita, KS*

MP 244 **Energy Deposition During Electron Ionization of Molecules**; Karl Irikura; *Natl Inst Standards & Tech, Gaithersburg, MD*

MP 245 **Theoretical Studies on Reactions of Gas Phase Ions with Water Covered α-quartz Surfaces**; Alexander Haack[1]; Walter Wissdorf[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal*

MP 246 **Developing a Fundamental Understanding of Inlet Ionization through Density Functional Theory (DFT)**; Wen-Jing Zhang[1]; Bishnu Thapa[1]; H. Bernhard Schlegel[1]; Sarah Trimpin[1]; *[1]Department of Chemistry, Wayne State University, Detroit, MI*

MP 247 **Theoretical Investigation of the Reactivity of para-Benzyne Ions Toward Cyclohexane in the Gas Phase**; Jacob R Milton[1]; Huaming Sheng[2]; Xin Ma[1]; John J Nash[1]; Hilkka I Kenttamaa[1]; *[1]Purdue University-Department of Chemistry, West Lafayette, IN; [2]Merck Department of Process and Analytical Chemistry, Rahway, NJ*

MP 248 **Peptide Ion Structure Investigation;From Conformational Space Sampling to Accurate CCS Calculation**; Samaneh Ghassabi Kondalaji[1]; Mahdiar Khakinejad[2]; Stephen J. Valentine[2]; Amirmahdi Tafreshian[2]; *[1]West Virginia University, Morgantown, wv; [2]West Virginia University, Morgantown, WV*

MP 249 **Stability of a Transient Protein Complex in a Charged Aqueous Droplet with Variable pH**; Styliani Consta; *London, ON, Canada*

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MP 250 **Selective Ion Ultraviolet Photodissociation (UVPD) Utilizing Ion Trap Resonance Excitation Modulation of Peptide and Protein Ions**; Dustin D Holden[1]; James D Sanders[1]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

MP 251 **Study on the Solvent Clusters' Effect on Ionization Efficiency of Polycyclic Aromatic Hydrocarbons by (+) Atmospheric Pressure Photoionization**; Seulgidaun Lee[1]; Arif Ahmed[1]; Sunghwan Kim[1]; *[1]Kyungpook National University, Daegu, South Korea*

MP 252 **Capture of Fleeting Amine Radical Cations and Elucidation of Chain Processes in Visible Light-Mediated [3+2] Annulation by Mass Spectrometry**; Yi Cai[1]; Jiang Wang[2]; Yuexiang Zhang[1]; Zhi Li[1]; Hao Chen[1]; Nan Zheng[2]; *[1]Ohio University, Athens, OH; [2]University of Arkansas, Fayetteville, AR*

MP 253 **REMPI and MATI Spectroscopy of Pyridine Derivatives**; Niklas Helle[1]; Sascha Krüger[1]; Tassilo Muskat[1]; Jürgen Grotemeyer[1]; *[1]Inst. f. Phys. Chem der CAU zu Kiel, Kiel*

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MP 255 **High Speed Analysis: Combining Fast GC with Time-of-Flight Mass Spectrometry for Complex Sample Analysis in Under One Minute**; Jonelle Shiel[1]; Matthew Soyk[2]; Aviv Amirav[3, 4]; Alex Fialkov[3]; Viatcheslav Artaev[2]; *[1]LECO Corporation, St. Joseph, MI; [2]LECO Corporation, St. Joseph, MI; [3]School of Chemistry, Tel Aviv University, Tel Aviv, Israel; [4]Aviv Analytical Ltd, Tel Aviv, Israel*

MP 256 **GCxGC-HRMS: Combining Multidimensional GC with Ultra High Resolution Time-of-Flight Mass Spectrometry for Comprehensive Analysis of Complex Samples**; Viatcheslav Artaev[1]; Scott J. Pugh[2]; George Tikhonov[2]; *[1]LECO Corporation, St Joseph, MI; [2]LECO Corporation, St. Joseph, MI*

MP 257 **Development and Application of a Sensitive Analytical Method for the Analysis of Cyanobacteria-Related Off-Flavor Compounds in Water using GC-MS/MS**; Morgan Solliec[1]; Benoit Barbeau[1]; *[1]Polytechnique Montréal - NSERC Industrial Chair on Drinking Water, Montréal, QC, Canada, Canada*

MP 258 **Improving the Chromatographic Capabilities of an Atmospheric Pressure Chemical Ionisation Source Coupled to a Gas Chromatograph**; Gareth Rhys Jones[1]; David Douce[1]; Richard Jarrold[1]; Anthony Hesse[1]; *[1]Waters Wilmslow UK, Wilmslow, Cheshire*

MP 259 **Online GCMS Measurement Method using Autosampler: SPME and Purge-Trap Technique**; Jaewon Choi[1]; Sung-Yun Ahn[1]; Wonkyung Lee[2]; Il-hwan Choi[1]; Yuns Kim[1]; *[1]Kwater, Daejeon, Daejeon; [2]Euro Science, Seoul, South Korea*

MP 260 **Evaluation of Field Ionization Source Parameters Using GCxGC-FI-TOFMS for Petroleum Distillate Fractions Analysis**; Hung Anthony Pham[1]; Wayne Rathbun[1]; Haiyan Wang[1]; Kendall Guyer[1]; *[1]UOP LLC, Des Plaines, IL*

MP 261 **Residual Solvents Analysis: Satisfying USP 467 Using a New Benchtop Time-of-Flight Mass Spectrometer**; Joe Binkley[1]; Christina Kelly[2]; Lorne Fell[1]; *[1]LECO Corporation, Saint Joseph, MI; [2]LECO Corporation, Saint Joseph, MI*

MP 262 **Japanese Lacquer Film Analysis by using Pyrolysis Comprehensive Two-Dimensional GC (Py/GCxGC) and High-Resolution TOFMS with Electron Ionization and Photoionization**; Masaaki Ubukata[1]; Jun Onodera[1]; Noriyasu Niimura[1]; Andrew John Dane[2]; Yoshimi Kamiya[3]; *[1]JEOL Ltd., Akishima, Japan; [2]JEOL USA Inc., Peabody, MA; [3]Tokyo Metropolitan Industrial Technology Research Institute, Akishima, Japan*

MP 263 **Estimation of Elemental Compositions for Additives in Polymers using Newly Developed EI/CI Ion Source without Venting MS**; Yukihiko Kudo[1]; Riki KItano[2]; Yoshiro Hiramatsu[1]; Yuki Sakamoto[1]; Katsuhiro Nakagawa[1]; Haruhiko MIyagawa[1]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Shimadzu Scientific Instruments, Columbia, MD*

MP 264 **The Analysis of All 209 PCB Isomers using GC-APCI-MS/MS at Selected Collision Energies and Correlation with Toxicity**; Jerry Hart[1]; Gareth Rhys Jones[2]; Malcolm Clench[1]; *[1]BMRC, Sheffield Hallam University, Sheffield, UK; [2]Waters Corporation, Wilmslow, UK*

MP 265 **Interleaving Ionisation Energy for Enhanced Confidence in the Identification of Fragrance Allergens**; Pete Grosshans[1]; Natasha Spadafora[1]; Matthew Edwards[2]; Laura McGregor[1]; Chris Hall[1]; Nick Bukowski[1]; *[1]Markes International, Llantrisant , Cardiff; [2]SepSolve Analytical, Peterborough, UK*

MP 266 **Coupling of Microfabricated GC Columns with a High Pressures Ion Trap Mass Spectrometer**; Yury Desyaterik[1]; John Perry[1]; Tina E. Stacy[1]; Jean Pierre Alarie[1]; Kevin Schultze[2]; J. Michael Ramsey[1]; *[1]UNC Chapel Hill, Chapel Hill, NC; [2]908 Devices Inc., Boston, MA*

MP 267 **Tandem Vacuum Ultraviolet Spectroscopy and Mass Spectrometry for Improved Identification of GC-Eluting Species**; Ian G. M. Anthony[1]; Matthew R. Brantley[1]; Christina A. Gaw[1]; Adam R. Floyd[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

MP 268 **Using Low Electron Energy Automatic Tuning to Increase High Mass Sensitivity on Orbitrap GC/MS**; Xin Zheng[1]; Jason Cole[1]; Brody Guckenberger[1]; Deven Shinholt[1]; Cristian Cojocariu[2]; Paul Silcock[2]; *[1]Thermo Fisher Scientific, Austin, TX; [2]Thermo Fisher Scientific, Runcorn, UK*

MP 269 **Applications for a Newly Developed Miniature GC-MS System**; Kevin P Schultze[1]; James A Roush[1]; Emily E Dunn[2]; Andrew C McDowell[1]; Scott E Miller[1]; *[1]908 Devices Inc., Boston, MA; [2]Northeastern University , Boston, MA*

MP 270 **Analysis of Pesticides and Environmental Pollutants in Essential Oil Using Multi-Platform GC/SQ, GC/TQ and GC/Q-TOF**; Vivian Xianyu Chen[1]; Kai Chen[2]; Bruce Quimby[3]; Andy Zhai[1]; *[1]Agilent Technologies, Shanghai, China; [2]Agilent Technologies, Santa Clara, CA; [3]Agilent Technologies, Wilmington, DE*

MP 271 **Reduction in EI Source Contamination: The Benefits of a Novel GC with an Inert Microfluidic Flow Path** ; Matthew Giardina[1]; Rebecca Veeneman[2]; *[1]Agilent Technologies, Inc, Wilmington, DE; [2]Agilent Technologies, Inc., Wilmington, DE*

MP 272 **Use of Methylamine PICI for Qualitative Analysis by GC/Q-TOF**; Ryo Ogasawara[1]; Sadao Nakamura[1]; *[1]Agilent Technologies Japan, Hachioji-shi, Tokyo*

MP 273 **Allergens in Perfume by GC/Q-TOF with a Low Energy EI Source**; Jennifer Sanderson[1]; Matthew Curtis[2]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]Agilent Technologies, Santa Clara, CA*

MP 274 **Analysis of Sulfur Containing Compounds in Heavy Matrices using Low Energy Electron Ionization**; Matthew Curtis[1]; Jennifer Sanderson[2]; *[1]Agilent Technologies, Santa Clara, CA; [2]Agilent Technologies, Inc., Santa Clara, CA*

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MP 275 **3D DESI-MS Lipid Imaging of a Xenograft Glioblastoma**; Fiona Henderson[1]; Emrys Jones[2]; Joanna Denbigh[3]; Lidan Christie[1]; Emmanuelle Claude[2]; Kaye J Williams[1]; Adam McMahon[1]; *[1]The University of Manchester, Manchester, UK; [2]Waters Corporation, Wilmslow, UK; [3]University of Salford, Salford, UK*

MP 276 **Direct Imaging and Profiling of Mycobacterium tuberculosis and Fungal Lipids within Infected Tissue Lesions by MALDI-MSI and Laser Capture Microdissection**; Brendan Prideaux[1]; Landry Blanc[1]; Veronique Dartois[1]; *[1]PHRI, Rutgers University, Newark, NJ*

MP 277 **Study of Changes in the Kidney's Lipid Profile in the Case of Obesity using MALDI-ToF Imaging and ESI LC-MS-MS Analysis**; Gianluca Sighinolfi[1]; Daniela Cota[2]; Marc Bonneu[1]; Jean-Marie Schmitter[1]; Boutayna Rhourri-Frih[1]; *[1]CBMN, Bordeaux, France; [2]Inserm, Bordeaux, France*

MP 278 **Age-dependent Shift in Ganglioside Abundance Detected in Transgenic APP Rats using MALDI Imaging Mass Spectrometry**; Sarah Caughlin[1]; Shikhar Maheshwari[2]; Ken K.-C. Yeung[2]; David F. Cechetto[2]; Shawn N. Whitehead[3]; *[1]Western University, London, Ontario; [2]University of Western Ontario, London, ON, Canada ; [3]University of Western Ontario, London, ON, Canada*

MP 279 **Analysis of the Probiotics Effect on Bowel Inflammation by MALDI-ToF Imaging and LC-MS-MS**; Stefania Pozzan[1]; Maria Urdaci[1]; Mohamed Mokrani[1]; Marc Bonneu[1]; Jean-Marie Schmitter[1]; Boutayna Rhourri-Frih[1]; *[1]CBMN, Bordeaux, France*

MP 280 **MALDI Imaging Mass Spectrometry of Lipids in Nevi**; Jone Garate[1]; Veronica Velasco[2, 3]; Roberto Fernandez[1]; Sergio Lage[1]; Beatriz Abad[1]; Maria Angeles Rodriguez[1]; Aintzane Asumendi[1, 3]; Jesus Gardeazabal[2, 3]; Juan Antonio Raton[2, 3]; Begoña Ochoa[1]; Maria Dolores Boyano[1, 3]; Jose A. Fernandez[4]; *[1]Universidad del Pais Vasco, Leioa, Spain; [2]Cruces University Hospital, Barakaldo, Spain; [3]Biocruces Research Institute, Barakaldo, Spain; [4]Universidad del Pais Vasco, leioa, Spain*

MP 281 **Differentiating Macrophages in Atherosclerotic Plaques using Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry Imaging**; Pegah Khamehgir-Silz[1]; Florian Schnitter[2]; Su Hwan Kim[2]; Andreas H. Wagner[2]; Stefanie Gerbig[1]; Sabine Schulz[1]; Markus Hecker[2]; Bernhard Spengler[1]; *[1]Justus Liebig University Giessen, Giessen, Germany; [2]University of Heidelberg, Heidelberg, Germany*

MP 282 **Imaging of Lipid Distribution in a Metastatic Breast Cancer Mouse Model**; Shelley N Jackson[1]; Ludovic Muller[1]; Aurélie Roux[1]; Marise Heerma van Voss[2]; Venu Raman[2]; Amina S. Woods[1]; *[1]NIDA-IRP, NIH, Baltimore, MD; [2]Johns Hopkins University School of Medicine, Baltimore, MD*

MP 283 **High-Spatial Resolution Nanospray Desorption Electrospray Ionization Mass Spectrometry Imaging of Mouse Pancreatic Islets**; Ruichuan Yin[1]; Lori Sussel[2]; Jennifer Kyle[1]; Kristin Burnum-Johnson[1]; Charles Ansong[1]; Julia Laskin[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Barbara Davis Center for Diabetes, University of Colorado, Aurora, CO*

MP 284 **Imaging Regiospecific Lipid Turnover in Mouse Brain with Desorption Electrospray Ionization Mass Spectrometry**; Richard H Carson[1]; Charlotte Lewis[1]; Mercede N Erickson[1]; Paul B Farnsworth[1]; John Price[1]; *[1]Brigham Young University, Provo, UT*

MP 285 **Alcohol Consumption during Gestation Period Alters Phosphatidylcholine and Phosphatidylethanolamine Distribution in Developing Fetal Brain**; Aafreen Kaur Bagga[1]; Paige Whyte-Fagundes[1]; Georg R. Zoidl[1]; Demian R. Ifa[1]; *[1]York University, Toronto, ON, Canada*

MP 286 **A Multi-Center Study Using Desorption Electrospray Ionization Mass Spectrometry Imaging as A Robust Tool for Breast Cancer Diagnosis**; Jialing Zhang[1]; Andréia M Porcari[2]; Raquel R Peres[2]; Kyana Garza[1]; Jonathan Young[1]; John Lin[1]; Rob Tibshirani[3]; Geisilene R Paiva[2]; Wendong Yu[4]; Chandandeep Nagi[4]; Stacey Carter[4]; Luís Z Sarian[2]; Marcos N. Eberlin[2]; Livia S. Eberlin[1]; *[1]The University of Texas, Austin, TX; [2]State University of Campinas, Campinas, Brazil; [3]Stanford University, Stanford, CA; [4]Baylor College of Medicine, Houston, TX*

MP 287 **Nano-DESI Imaging for Detection of oxidative stress response associated to the Neurotoxicant Paraquat Exposure in Parkinson's Like Disease Animal Model**;

Son N. Nguyen[1]; Ryan Sontag[1]; Jordan Smith[1]; Charles Timchalk[1]; Julia Laskin[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

MP 288 **Tissue Mass Spectrometry Imaging Enabled Mapping of Sandhoff Biomarkers in Mouse Brain**; Walter Korfmacher[1]; Cristina Silvescu[1]; Hanlan Liu[1]; John Marshall[2]; Jennifer Nietupski[2]; Dinesh Bangari[2]; Susan Ryan[2]; Petra Oliva[2]; Thomas O'Shea[1]; *[1]Sanofi, Waltham, MA; [2]Sanofi, Framingham, MA*

MP 289 **Mass Spectrometry Imaging of Lipids in Niemann-Pick Disease C1**; Fernando Tobias[1]; Abraham Abraham[1]; Stephanie M Cologna[1]; *[1]University of Illinois at Chicago, Chicago, IL*

MP 290 **Molecular Characterization and Diagnosis of Endometriosis to Aid in Surgical Resection using Ambient Ionization Mass Spectrometry**; Clara Feider[1]; Suzanne Ledet[2]; Michael T. Breen[2]; Livia S. Eberlin[1]; *[1]University of Texas at Austin, Austin, TX; [2]Seton Medical Center, Austin, TX*

MP 291 **Identification of Biomarkers for Mild Traumatic Brain Injury in Tissue and Biological Fluids using DESI and PaperSpray Ionization with HRAM**; Joseph H Kennedy[1]; Riyi Shi[2]; Marcela Cruz-Haces[2]; Jonathan Tang[2]; Brian Laughlin[1]; Justin wiseman[1]; *[1]Prosolia, Inc., Indianapolis , IN; [2]Purdue University, West Lafayette, IN*

MP 292 **MALDI-FTICR Mass Spectrometry Imaging Reveals Dysregulated Metabolites in the Brains of Zika Virus Infected Mice**; Lisa H. Cazares[1, 2]; Darci R. Smith[2]; Bradley Hollidge[2]; Xiankun Zeng[2]; Candace Blancett[2]; Tara Kenny[2]; Connie Schmaljohn[2]; Sina Bavari[2]; *[1]Henry M. Jackson Foundation, Frederick, MD; [2]U.S. Army Medical Research Institute of Infectious Disease, Ft. Detrick, MD*

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MP 294 **High Spatial and Mass Resolution MALDI- Imaging Mass Spectrometry of Rat Optic Nerve Glial Scar Tissue**; David M. G. Anderson[1]; David T. Stark[2]; Nathan Heath Patterson[1]; Jacky M. Kwong[2]; Kevin L. Schey[1]; Joseph Caprioli[2]; Richard M. Caprioli[1]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Stein Eye Institute, Los Angeles, CA*

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MP 296 **Multi-Modal Imaging: Fusing Mass Spectrometry Imaging and Second Harmonic Generation to Understand Molecular Signatures and Collagen Alignment in Pancreatic Cancer**; Jillian Johnson[1]; Adib Keikhosravi[2]; Catherine Pearce[1]; Matthew Huppert[1]; Kevin Eliceiri[2]; Melissa Skala[2]; W. John Kao[3]; Lingjun Li[1, 4]; *[1]School of pharmacy, University of Wisconsin Madison, Madison, WI; [2]Department of Biomedical Engineering, University of Wisconsin-Madison, Madison, WI; [3]President's Office, The University of Hong Kong, Pokfulam, Hong Kong; [4]Department of chemistry, University of Wisconsin Madison, Madison, WI*

MP 297 **Exploration of Desorption Electrospray Ionization (DESI) and Touch Spray (TS) Mass Spectrometry for Squamous Cell Carcinoma (SCC) Diagnosis and Prognosis**; Cedric DHue[1]; Michael Moore[2]; Don-John Summerlin[3]; Alan Jarmusch[4]; R. Graham Cooks[5]; *[1], West Lafayette, IN; [2]University of California, Davis, Davis, CA; [3]Indiana University-Purdue University Indianapolis, Indianapolis, IN; [4]University of California, San Diego, San Diego, CA; [5]Purdue University, West lafayette, IN*

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MP 304 **MALDI Mass Spectrometry Imaging Investigation of Chemico-Spatial Composition of the Parathyroid Gland**; Qiyao Li[1]; Stanislav S Rubakhin[1]; Robyn E Ellerbrock[1]; Brian M Aldridge[1]; Adam C Puche[2]; Iris Lindberg[2]; Jonathan V Sweedler[1]; *[1]University of Illinois at Urbana Champaign, Urbana, IL; [2]University of Maryland School of Medicine, Baltimore, MD*

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MP 306 **Top-down Neuropeptide MALDI Imaging MS on FFPE Sections with High Mass Resolution and MS/MS Capabilities: Towards True "Mass Spectrometry Histochemistry"**; Peter D. Verhaert[1]; Shane R. Ellis[2]; Martin R. L. Paine[2]; Dan Maloney[3]; Ron MA Heeren[2]; *[1]Delft University of Technology, DELFT, Europe; [2]Maastricht Multi-Modal Molecular Imaging (M4I) Institute, Maastricht University, Maastricht, Netherlands; [3]Bioinformatics Solutions Inc, Waterloo, ON, Canada*

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MP 313 **Protein Identification without Peptide Identification**; Jamie Sherman[1]; Stephen Tate[2]; *[1]SCIEX, Concord, ON, Canada; [2]SCIEX, Concord, ON, Canada*

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MP 324 **Evaluating the Impact of Multiple Search Engines and De-novo Sequencing Algorithms for Obtaining Deeper Proteome Coverage in Complex Environmental Samples**; Ramsunder Iyer[1, 2]; Robert L Hettich[2]; *[1]University of Tennessee, Knoxville, TN; [2]Oak Ridge National Laboratory, Oak Ridge , TN*

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Fabien Fontaine[2]; Luca Morettoni[5]; *[1]Universitat Pompeu Fabra, Barcelona, Spain; [2]Lead Molecular Design, S.L., Sant Cugat del Valles, Spain; [3]Merck & Co., West Point, PA; [4]Pharmaceutical Sciences, Pharma Research and Early Development, Roche Innovation Center Basel F. Hoffmann-La Roche Ltd., Basel, Switzerland; [5]Molecular Discovery, London, UK*

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MP 334 **Towards a m/z Unlimited Algorithm for Peptide and Protein Structure Elucidation**; Fabien Fontaine[1, 2]; Ismael Zamora[1, 3]; Christopher Kochansky[4]; *[1]Lead Molecular Design, S.L., Sant Cugat del Valles, Spain; [2]Molecular Discovery, London, UK; [3]Pompeu Fabra University, Barcelona, Spain; [4]Merck & Co., West Point, PA*

MP 335 **Identifying Co-Eluting Peptides using MS Amanda and Elutator**; Viktoria Dorfer[1]; Sergey Maltsev[2]; Stephan Winkler[1]; Karl Mechtler[2, 3]; *[1]University of Applied Sciences Upper Austria, Hagenberg, AUT; [2]Research Institute of Molecular Pathology (IMP), Vienna, Austria; [3]Institute of Molecular Biotechnology, Vienna, Austria*

MP 336 **PeptidePicker Version 2: Selecting Suitable Proteotypic Peptides for Targeted Proteomics Experiments**; Yassene Mohammed[1, 2]; Pallab Bhowmick[1]; Christoph H. Borchers[1, 3, 4]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Center for Proteomics and Metabolomics, Leiden University, Netherlands; [3]Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; [4]Dept. of Oncology, Segal Cancer Centre, Jewish General Hospital, McGill University, Montreal, QC, Canada*

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MP 340 **DeltaMass: Analysis and Viewer Software for Examining Wide Precursor Window Search Results in Proteomics**; Dmitry M. Avtonomov[1]; Andy Kong[1]; Alexey I. Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI*

MP 341 **Improvements to Protein Prospector's MS-Viewer**; Peter R Baker[1]; Carolyn Chitty[2]; Robert J Chalkley[2]; *[1]UCSF, Rokietnica; [2]UCSF, San Francisco, CA*

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MP 344 **Molecular-beam Mass Spectrometric and Numerical Investigation of the Intrusive Flame Sampling Effect on Premixed Low-Pressure Flame Structure**; Yasin Karakaya[1]; Lei Deng[1]; Irenäus Wlokas[1]; Martin Höner[1]; Tina Kasper[1]; *[1]University of Duisburg-Essen, Duisburg, Germany*

MP 345 **Sample Flow Rate Scan in Mass Spectrometry**; Gurpur Rakesh D. Prabhu[1]; Pawel L. Urban[1]; *[1]National Chiao Tung University, Hsinchu, Taiwan*

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MP 348 **Analytical Tool for the Study of Collection Efficiency of Explosives from Surfaces** ; Vladimir Romanov[1]; Steven Watt[1]; Thomas Hagerty[1]; Hartwig Schmidt[1]; Stefan Lukow[1]; *[1]Morpho Detection, Andover, MA*

MP 349 **Accessing High Performance Microflow on a Chip-Based Platform**; Helena Svobodova[1]; Aaron Dewberry[1]; Amanda Berg[1]; Mike S. Lee[2]; Gary Valaskovic[1]; *[1]New Objective, Woburn, MA; [2]Milestone Development Services, Inc., Newtown, PA*

MP 350 **Open-Port Probe Sampling Interface for the Direct Coupling of Solid-Phase Microextraction to Atmospheric Pressure Ionization Mass Spectrometry**; Chang Liu[1]; Germán Gómez-Ríos[2]; Marcos Tascon[2]; Bradley B Schneider[1]; Nathaly Reyes-Garcés[2]; Don W Arnold[3]; Thomas R. Covey[1]; Janusz Pawliszyn[2]; *[1]SCIEX, Concord, ON, Canada; [2]University of Waterloo, Waterloo, Ontario; [3]SCIEX, Redwood City, CA*

MP 351 **Front-end Developments for Trace Analyte Collection, Desorption, and Ionization of Vapor and Particulate Species**; Thomas P. Forbes[1]; Matthew Staymates[1]; Edward Sisco[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

MP 352 **High-Throughput Mass Spectrometry: Direct Acoustic Ionization for Sub-Second Sample Processing in Biochemical Screens**; Lucien Ghislain[1]; Martin Bachman[2]; Ian Sinclair[2]; Jonathan Wingfield[3]; Daniel Addison[2]; Eric Hall[1]; Rick Stearns[1]; Lars Majlof[1]; Richard Ellson[1]; Gareth Rhys Jones[4]; Emmy Hoyes[4]; Steven Derek Pringle[4]; Sammy Datwani[1]; *[1]Labcyte Inc, Sunnyvale, CA; [2]AstraZeneca R&D, Alderley Park, UK; [3]Astrazeneca, Cambridge, UK; [4]Waters Corporation, Wilmslow, UK*

MP 353 **The T-probe: A Novel Device for Rapid MS Analysis of Non-Adherent Live Single Cells**; Yanlin Zhu[1]; Renmeng Liu[1]; Zhibo Yang[1]; *[1]The University of Oklahoma, Norman, OK*

MP 354 **High-throughput (sub-2.5 second) Direct Injection using a Modified RapidFire 365 HTMS System**; Peter Rye[1]; Arrin Katz[2]; William LaMarr[2]; Can Ozbal[2]; *[1]Agilent, Lexington, MA; [2]Pure Honey Technologies, Billerica, MA*

MP 355 **Development of a Mass Spectrometry Cartridge for Plasma Protein Analysis with integrated Antibody Column and Spray Substrate**; Chengsen Zhang[1]; Nicholas E. Manicke[1]; *[1]Indiana University−Purdue University Indianapolis, Indianapolis, IN*

MP 356 **Polymer-Coated Capillary Sampler for Direct Mass Spectrometry Quantitation of Fatty Acids in Biofluids**; Wenpeng Zhang[1, 2]; Spencer Chiang[1]; Yu Xia[2]; Zheng Ouyang[1, 2, 3]; *[1]Weldon School of Biomedical Engineering, Purdue University, West Lafayette, Indiana; [2]Department of Chemistry, Purdue University, West Lafayette, IN; [3]Tsinghua University, Beijing, Beijing*

MP 357 **Robotic Surface Analysis Mass Spectrometry (RoSA-MS)**; Anyin Li[1]; Martin R. L. Paine[1]; Rachel V Stryffeler[1]; Jason Wu[1]; Stephen Zambrzycki[1]; Jake Huckaby[2]; Chu-yin Change[2]; Manoj Kumar[2]; Piyoosh Mukhija[2]; Alexander S Lambert[1]; Ruffin J White[1]; Henrik I Christensen[1]; Facundo M Fernandez[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]Energid, Cambidge, MA*

MP 358 **Droplet Based Sampling of RNA Hydrolysates by Induction Based Fluidics**; Robert Ross[1]; Manasses Jora[1]; Andrew D. Sauter III[2]; Drew Sauter[2]; Patrick A. Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH; [2]Nanoliter, LLC, Henderson , NV*

MP 359 **Atomic Force Microscope Mediated Thermal Microsampling with Atmospheric Pressure Temperature Ramped Thermal Desorption/Ionization – Mass Spectrometry Analysis**; William D. Hoffmann[1]; Vilmos Kertesz[1]; Gary J. Van Berkel[1]; *[1]Oak Ridge National Laboratory, Oak Ridge , TN*

MP 360 **Ambient Submicron Sampling of Biological Samples by Combining AFM with MS**; Jonathan Brauer; *Anasys Instruments, Santa Barbara, CA*

MP 361 **Programmable Stage for Fluorescence-Guided Atmospheric Pressure Mass Spectrometry Imaging of Frozen Tissue Sections by Laser Ablation Electrospray Ionization**; Rikkita Khattar[1]; Sylwia A Stopka[1]; Beverly J Agtuca[2]; Christopher R Anderton[3]; David W. Koppenaal[3]; Ljiljana Pasa-Tolic[3]; Gary Stacey[2]; Akos Vertes[1]; *[1]George Washington University, Washington, DC; [2]University of Missouri, Columbia, MO; [3]Pacific Northwest National Laboratory, Richland, WA*

MP 362 **Liquid Chromatography-Plasma Assisted Reaction Chemical Ionization Mass Spectrometry for the Analysis of Chlorinated Compounds**; Joseph Lesniewski[1]; Kunyu Zheng[1]; William McMahon[1]; Hamid Badiei[2]; Heng Keang Lim[3]; Kaveh Jorabchi[1]; *[1]Georgetown Univ., Washington, DC; [2]PerkinElmer Inc, Shelton, CT; [3]Janssen Research&Development, Spring House, PA*

MP 363 **Application of an Acoustic Interface for Ultra-High-Throughput Mass Spectrometry in Drug Discovery**; ian Sinclair[1]; Martin Bachman[2]; Jonathan Wingfield[3]; mattias rohman[4]; Lucien Ghislain[5]; Eric Hall[5]; Gareth Rhys Jones[6]; Michael Morris[6]; Richard Ellson[5]; Rick Stearns[5]; *[1]AstraZeneca, macclesfield, Cheshire; [2]AstraZeneca R&D, Alderley Park, UK; [3]Astrazeneca, Cambridge, UK; [4]Astrazeneca, Mölndal, Mölndal; [5]Labcyte Inc, Sunnyvale, CA; [6]Waters Corporation, Wilmslow, UK*

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MP 364 **Variable-velocity Traveling-wave Ion Mobility Separation Enhances Peak Capacity for Data-independent Acquisition Proteomics**; Sarah E. Haynes[1]; Daniel A. Polasky[1]; Sugyan M. Dixit[1]; Jaimeen D. Majmudar[1]; Brandon T. Ruotolo[1]; Brent R. Martin[1]; *[1]University of Michigan, Ann Arbor, MI*

MP 365 **Impact of Ion Focusing Parameters on Transmission and Fragmentation of Coordination Driven Self-Assembly Product Ions**; Christopher S. Mallis[1]; Manik L. Saha[2]; Peter J. Stang[2]; David H. Russell[1]; *[1]Texas A&M University, College Station, TX; [2]University of Utah, Salt Lake City, UT*

MP 366 **Simulation of a Novel Annular Geometry Ion Mobility Trap and Separation Device with High Space Charge Capacity**; David Langridge[1]; Martin Green[1]; Kevin Giles[1]; *[1]Waters Corporation, Wilmslow, UK*

MP 367 **Measuring Precise Collision Cross Section Values from Liquid Chromatography Ion Mobility Tandem Mass Spectrometry Experiments**; Charles M. Nichols[1]; Sarah M. Stow[2]; Jaqueline A. Picache[1]; Jody C. May[1]; Stacy D. Sherrod[1]; John Fjeldsted[2]; John A. McLean[1]; *[1]Vanderbilt University, Nashville, TN; [2]Agilent Technologies, Santa Clara, CA*

MP 368 **Ion Separation in Air Using a 3D Printed Ion Mobility Spectrometer**; Adam Hollerbach[1]; Zane Baird[2]; Graham Cooks[1]; *[1]Purdue University, West Lafayette, IN; [2]Present address: Indiana Biosciences Research Institute, Indianapolis, IN*

MP 369 **Ion Mobility Support in a Novel Compound-Centric Database and Accurate Mass Spectral Library**; Emma E Rennie[1]; Kristina L Milkovich[1]; Norton Kitagawa[1]; Mahsan Miladi[1]; Crystal K Cody[1]; Stephen Madden[1]; Nagapadmini Pavuluri[1]; John C Fjeldsted[1]; *[1]Agilent Technologies Inc., Santa Clara, CA*

MP 370 **Quadrupole Wide Band Isolation Directed by Ion Mobility Drift Separation in Metabolomics Experiments**; Teresa Mairinger[1]; Ruwan Kurulugama[2]; Tim Causon[1]; George Stafford[3]; John Fjeldsted[3]; Stephan Hann[1]; *[1]University of Natural Resources and Life Sciences - BOKU, Vienna, Austria; [2]Agilent Technologies Inc., Santa Clara, CA; [3]Agilent Technologies, Inc., Santa Clara, CA*

MP 371 **Synchronizing Ion Mobility with Quadrupole Mass Filtering for Highly Efficient Background Removal during Acquisition for Metabolite Identification**; Jayne Kirk[1]; Darren Hewitt[1]; Martin Palmer[1]; Jason wildgoose[1]; Mark Wrona[2]; *[1]Waters Corp., Wilmslow, UK; [2]Waters Corp, Milford, MA*

MP 372 **The Use of SelexION to Increase Sensitivity for Trace Level Analysis of Small Molecules**; Christopher Borton[1]; Paul C. Winkler[1]; Jay Jones[2]; *[1]SCIEX, Framingham, MA; [2]BASF, Research Triangle Park, NC*

MP 373 **Building a Collision Cross Section Library of Pharmaceutical Drugs using an IMS QTof Platform** ; Yun Alelyunas[1]; Kerri Smith[2]; Russell Mortishire-Smith[2]; Mark D. Wrona[2]; Nigel Ewing[2]; *[1], Milford, MA; [2]Waters Corp, Milford, MA*

MP 374 **Development of a SUPER SLIM TWIM-MS Application Platform for Multi-Omics Analysis**; Christopher D Chouinard[1]; Ian K Webb[1]; Spencer A Prost[1]; Yehia M Ibrahim[1]; Liulin Deng[1]; Xueyun Y Zheng[1]; Randolph V Norheim[1]; Colby E Schimelfenig[1]; Erin S Baker[1]; RICHARD D. SMITH[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

MP 375 **Influence of Ionization Source Conditions on Protomer, or Deprotomer Ratios of Multifunctional Gaseous Ions Demonstrated by Ion Mobility Mass Spectrometry**; Athula B. Attygalle; *Stevens Institute of Technology, Hoboken, NJ*

MP 376 **High-throughput, Charge-multiplexed Collision-induced Unfolding Measurements for Rapid Biotherapeutic Analysis**; Joseph D Eschweiler[1]; Ruwan Kurulugama[2]; John Fjeldsted[2]; Brandon T Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI; [2]Agilent Technologies, Santa Clara, CA*

MP 377 **Characterization of the Interaction Between microRNA 122 and Hepatitus C Viral RNA**; Cesar Masitas[1]; Jonathan Trinidad[1]; *[1]Indiana University Bloomington, Bloomington, IN*

MP 378 **Separation of Isobaric Phospholipids and Fatty Acids Derived from Murine Adipose Tissue using Ion Mobility Coupled with High-Resolution Mass Spectrometry**; Christine Hinz[1]; Sonia Liggi[1]; Julia Denes[1]; Antonio Murgia[1, 2]; Zoe Hall[1]; Ke-di Liu[1]; John Fjeldsted[3]; Julian L. Griffin[1]; *[1]University of Cambridge, Cambridge, UK; [2]Università degli Studi di Cagliari, Cagliari, Italy; [3]Agilent Technologies, Santa Clara, CA*

MP 379 **Extractive Electrospray Ionization Coupled to Atmospheric Pressure DTIMS-MS for Real-Time Analysis of Aerosols**; Paul S. Soma[1]; Kenneth D. Swanson[1]; Gary L. Glish[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC*

MP 380 **Non-Enzymatic Stepwise Degradation of Substance P Measured by Hybrid IMS-MS**; Christopher R. P. Conant[1]; Daniel R Fuller[1]; Alison E Holliday[2]; David H Russell[3]; David E Clemmer[1]; *[1]Indiana University Bloomington, Bloomington, IN; [2]Moravian College, Bethlehem, Pennsylvania; [3]Texas A&M University, College Station, TX*

MP 381 **Evidence for a Globule to Helix Gas-Phase Transition in an α-Synuclein Peptide Segment**; Goran Tumbic[1]; Michael Przybylski[2]; David E Clemmer[1]; *[1]Indiana University Bloomington, Bloomington, IN; [2]Steinbeis Centre Biopolymer Analysis and Biomedical Mass Spectrometry, Ruesselsheim am Main, Germany*

MP 382 **Examining the Structural Influence of Site Specific Phosphorylation by Ion Mobility-Mass Spectrometry**; Rebecca S. Glaskin[1]; Caroline S. Chu[2]; *[1]Agilent Technologies, Inc., Wilmington, DE; [2]Agilent Technologies, Inc., Santa Clara, CA*

MP 383 **Large Scale Collision Cross Section (CCS) Profiling of Endogenous Neuropeptides by Ion Mobility Mass Spectrometry**; Zichuan Tian[1]; Zhengwei Chen[2]; Matthew Glover[3]; Qinjingwen Cao[4]; Lingjun Li[4, 5]; *[1], Madison, WI; [2]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [3]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [4]Department of chemistry, University of Wisconsin Madison, Madison, WI; [5]School of pharmacy, University of Wisconsin Madison, Madison, WI*

MP 384 **Simultaneous Tracking of Individual Protein Stabilities in a Mixture by Ion Mobility Spectrometry-Mass Spectrometry**; Kyle Buckley[1]; Tarick El-Baba[1]; Daniel W Woodall[1]; David E Clemmer[1]; *[1]Indiana University Bloomington, Bloomington, IN*

MP 385 **Assessment of Dimeric Metal-Glycan Adducts via Isotopic Labeling and Ion Mobility-Mass Spectrometry**; Kelsey A. Morrison[1]; Brad K. Bendiak[2]; Brian Clowers[1]; *[1]Washington State University, Pullman, WA; [2]University of Colorado Health Sciences Center, Aurora, CO*

MP 386 **Visualizing and Conceptualizing Highly-Dimensional Metabolomics Data from LC-IM-MS/MS Analysis**; Jaqueline A. Picache[1]; Charles M. Nichols[1]; John C. Fjeldsted[2]; Stacy D. Sherrod[1]; Jody C. May[1]; John A. McLean[1]; *[1]Vanderbilt University, Nashville, TN; [2]Agilent Technologies Inc., Santa Clara, CA*

MP 387 **Probing Supramolecular Assembly Processes by Ion Mobility Mass Spectrometry**; Kevin J Endres[1]; George R Newkome[1]; Chrys Wesdemiotis[1]; *[1]The University of Akron, Akron, OH*

MP 388 **Structural Database of Secondary Metabolites: Conformational Mapping using Ion Mobility-Mass Spectrometry as a Tool for Natural Product Discovery**; Andrzej Balinski[1]; John A. McLean[2]; Jody C. May[2]; Brian O. Bachmann[2]; Sarah M. Stow[3]; *[1]Vanderbilt University, Nashville, TN; [2]Vanderbilt University, Nashville, TN; [3]Agilent Technologies Inc., Santa Clara, CA*

MP 389 **Differential Analysis of 4-dimensional LC-IMS-MS Data in the Analysis of Complex Samples**; Niels Goedecke[1]; Peter Sander[1]; Sven Meyer[1]; Klaus Meyer[1]; *[1]Bruker Daltonik GmbH, Bremen, Germany*

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MP 390 **SCX Contamination: A New Class of Pan-Assay Interference Compounds (PAINS)?**; Kenneth Roth[1]; Phillip Sanders[1]; Brandon Margolis[1]; *[1]Eli Lilly & Co., Indianapolis, IN*

MP 391 **Analysis of Commercially Available Beta-Glucuronidase Enzymes and Optimum Hydrolysis Conditions in Urine for Licit and Illicit Drugs using In-Well Hydrolysis**; Jillian Neifeld[1]; Dan Menasco[1]; Stephanie J Marin[1]; Bruce Kempf[1]; Helen Lodder[2]; Alan Edgington[2]; Adam Senior[2]; Paul Roberts[2]; Lee Williams[2]; Elena Gairloch[1]; Claire Desbrow[2]; Steve Jordan[2]; *[1]Biotage, Charlotte, NC; [2]Biotage GB Limited, Cardiff*

MP 392 **Fractionation of Whole Gut Lavage Fluid by Affinity Immunoglobulin Alpha Depletion for Increased Proteomic Coverage**; Joseph Otto[1]; Jana M Rocker[1, 2]; Lewis K. Pannell[1]; *[1]Mitchell Cancer Inst, Mobile, AL; [2]Mississippi Gulf Coast Community College, Gulfport, MS*

MP 393 **Evaluation of Recombinant, Chemically Treated Trypsin in Proteomics and Protein Characterization Assays**; Nicolas Caffarelli[1]; Judy Boland[1]; Jeff Turner[1]; Gordon Nicol[1]; Amber Henry[1]; Kevin Ray[1]; *[1]MilliporeSigma, St. Louis, MO*

MP 394 **Factors Effecting the Quality of FASP-prepared Proteomics Samples**; Shekufeh Zareian[1]; Michael J Sweredoski[1]; Sonja Hess[1]; Annie Moradian[1]; *[1]Caltech, Pasadena, CA*

MP 395 **Analysis of Per/Polyfluoroalkyl Substances (PFASs) in Biological Fluid using a Novel Lipid Removing Sorbent and LC/MSMS**; joan stevens[1]; Xiaomi Xu[1]; Tarun Anumol[1]; Limian Zhao[1]; *[1]Agilent Technologies, Inc., Wilmington, DE*

MP 396 **Automated Peptide Desalting using Dispersive Pipette Extraction Tips for Increased Protein Identifications**; Sunil Hwang[1]; Todd Mullis[1]; Michael Mouridian[2]; Andrew Lee[1]; *[1]IMCS, Columbia, South Carolina; [2]Hamilton Robotics, Reno, NV*

MP 397 **LC-MS/MS Method for the Determination of25-hydroxyvitamin D2/D3from Serum Sample using CleanertSLE**; Suzi Qin[1]; Qun Wang[1]; Wan Wang[1]; Warren Chen[1]; *[1]Bonna Agela Technologies, Tianjin, China*

MP 398 **LC-MS Analysis of Reserpine Using High pH Buffer** ; Subhra Bhattacharya[1]; Stephen C Roemer[2]; *[1]Thermo Fisher Scientific, Fair Lawn, NJ; [2]Thermo Fisher Scientific, Fair Lawn, NJ*

MP 399 **Comparison of Three Sample Preparation Methods for Determining Perfluoroalkyl Substances, Feminizing Compounds, and Mycotoxins in Serum Using UPLC-MS/MS**; Yen-Chun Liu[1]; Shin-Hung Liu[1]; I-Jen Wang[2]; Pau-Chung Chen[3, 4]; Chia-Yang Chen[1, 4]; *[1]Institute of Environmental Health, National Taiwan University, Taipei City, Taiwan; [2]Department of Pediatrics, Taipei Hospital, Ministry of Health and Welfare, New Taipei City, Taiwan; [3]Institute of Occupational Medicine and Industrial Hygiene, National Taiwan University, Taipei City, Taiwan; [4]Department of Public Health, National Taiwan University, Taipei City, Taiwan*

MP 400 **Operational Impact on the Correlation of Bioanalytical Results Generated by Dried Blood Spot and Whole Blood Lysate Sampling**; Shenita Basdeo[1]; Qin Ji[2]; *[1], Lawrenceville, NJ; [2]BMS, Princeton, NJ*

MP 401 **A Recombinant Asp-Specific Protease for Bottom-up Mass Spectrometry Workflows**; Chris Hosfield[1]; James Hartnett[1]; Alba Katiria González Rivera[1, 2]; Ethan Strauss[1]; Sergei Saveliev[1]; Michael Rosenblatt[1]; Marjeta Urh[1]; *[1]Promega Corporation, Madison, WI; [2]University of Wisconsin Madison, Madison, WI*

MP 402 **A Novel Strategy for the In-Process Stabilization of N-Oxide Metabolites in Hemolyzed Plasma Determined by LC-MS/MS**; Richard Lavallee[1]; Georges Koudssi[1]; Milton Furtado[1]; Anahita Keyhani[1]; *[1]Altasciences, Laval , QC, Canada*

MP 403 **Comparison of Commonly used Anti-adsorptive Agents to Identify an Optimal Strategy to Minimize Non-specific Binding in CSF Collection**; Adam Amaral[1]; Stanley I. Goldstein[1]; Michael T Rooney[1]; *[1]Biogen, Cambridge, MA*

MP 404 **Analysis of Free and Encapsulated Doxorubicin by LC-MS/MS**; Roger Demers[1]; Ying Ren[2]; Daria L Wentzel[2]; *[1]Tandem Labs, West Trenton, NJ; [2]Covance, West Trenton, NJ*

MP 405 **Polymeric vs Diatomaceous Earth SLE Sorbents: A Comparison of Phospholipid Depletion, Matrix Effect and Recovery for Cortisol and 6β-Hydroxycortisol**; Laurence Mayrand Provencher[1]; Sylvain Latour[1]; Jeff Plomley[1]; Milton Furtado[1]; Anahita Keyhani[1]; *[1]Altasciences, Laval , QC, Canada*

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MP 406 **Phospholipid Characterization by a TQ-MS Dada Based Identification Scheme**; Tsuyoshi Nakanishi[1]; Masaki Yamada[1]; Ningombam Sanjib Meitei[2, 3]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]PREMIER Biosoft, Palo Alto, CA; [3]PREMIER Biosoft, Indore, India*

MP 407 **Using MALDI-Mass Spectrometry Imaging to Assess the Oxidative Damage to Lipids Induced by *in vivo* Hydroxyl Radical-Based Protein Footprinting**; Jessica A. Espino[1]; Claire L. Carter[1]; Maureen A. Kane[1]; Lisa M. Jones[1]; *[1]University of Maryland School of Pharmacy, Baltimore, MD*

MP 408 **Characterization of Cardiolipin and Monolysocardiolipin Acyl-Lipid Species in an Acute Myeloid Leukemia Cell Line**; Juan J Aristizabal Henao[1]; Ayesh K Seneviratne[2]; Richard W Smith[1]; Aaron D Schimmer[2]; Ken D Stark[1]; *[1]University of Waterloo, Waterloo, Ontario; [2]Princess Margaret Cancer Centre, Toronto, ON, Canada*

MP 409 **Comparative Analysis of Plasma Lipid Alterations Associated with Age and Dietary Restriction using Targeted MS and Untargeted LC-MS Lipidomics Approaches**; Kevin Contrepois[1]; Salah Mahmoudi[1]; Anne Brunet[1]; Michael Snyder[1]; *[1]Stanford University, Stanford, CA*

MP 410 **Comparative Lipidomic Profiling of Four Shellfishes by UPLC-HRMS**; Jie Xu[1, 2]; Yu Song[3]; Peixu Cong[3]; Changhu Xue[3]; *[1]Ocean University of China, Qingdao, China; [2]currently as a visiting professor at the School of Biological Sciences, Georgia Institute of Technology, Atlanta, GA; [3]College of Food Science and Engineering, Ocean University of China, Qingdao, China*

MP 411 **An Integrated Strategy for Gangioside Lipidomics utilizing HRMS and Skyline Software**; Asoka Ranasinghe[1]; Eugene Ciccimaro[2]; Celia D'Arienzo[2]; Serhiy Hnatyshyn[3]; Timothy Olah Timothy Olah[2]; *[1]Bristol-Myers Squibb Company, Princeton, NJ; [2]Bristol-Myers Squibb, Princeton, New Jersey; [3]Bristol-Myers Squibb, Princeton, NJ*

MP 412 **LC-MSE-driven Discovery of Biomarkers for Identifying Heightened Risk of Developing Atherosclerotic Disease**; Zifeng Song[1]; Gerd Bobe[1, 2]; Sahar Taqui[3]; Jan F. Stevens[1, 2]; Johathan Lindner[3]; Claudia S. Maier[1, 2]; *[1]Oregon State University, Corvallis, OR; [2]Linus Pauling Institute, Oregon State University, Corvallis, OR; [3]Oregon Health & Science University, Portland, OR*

MP 413 **Analyses of Lipid Hydroperoxides in HDL and LDL of Human using Orbitrap Mass Spectrometer**; Shu-Ping Hui[1]; Hitoshi Chiba[1]; *[1]Faculty of Health Sciences, Hokkaido University, Sapporo, Japan*

MP 414 **Lipidomic Studies of Beta-2-Adrenergic Receptor Agonist-induced Hepatic Steatosis in Mice**; Xiaoli Gao[1]; Yun Shi[1]; Dana M. Molleur[1]; Susan T. Weintraub[1]; Amrita Kamat[1]; *[1]UT Health San Antonio, San Antonio, TX*

MP 415 **Differential Ion Mobility Coupled to a Multi-emitter Nanoelectrospray Ion Source for Improved Shotgun Lipidomics Applications**; James E. Keating[1]; Gary L. Glish[1]; *[1]University of North Carolina at Chapel Hill, Department of Chemistry, Chapel Hill, NC*

MP 416 **Pilot Study of the Plasma Lipid Profile in Ebola Vaccinated Healthy Donors using Untargeted Lipidomics Approach**; Manoj Khadka; *Emory University School of Medicine, Atlanta, GA*

MP 417 **Mass Spectrometry-Based Characterization of Milk Lipids Isolated from Murrah Buffalo**; Kiran Ambatipudi[1]; Aparna Verma[1]; Sivaramaiah Nallapeta[2]; *[1]Indian Institute of Technology Roorkee, Roorkee, UK; [2]Bruker Daltonics India, Centre of Excellence, Bangalore, India*

MP 418 **Automated Lipid Profiling of Malaria Samples Using Orbitrap Velos Pro Mass Spectrometer with LipidSearch and SimLipid Software**; Ningombam Sanjib Meitei[1, 2]; Arun Apte[3]; Fatima Rahlouni[4]; David J. Sullivan[5]; Vladimir Shulaev[4]; *[1]PREMIER Biosoft, Palo Alto, CA; [2]PREMIER Biosoft, Indore, India; [3]PREMIER Biosoft, Indore, India; [4]University of North Texas, Denton, TX; [5]Bloomberg School of Public Health, Johns Hopkins University, Baltimore, MD*

MP 419 **Investigating Current Limitations and Pitfalls in Lipidomics using the SRM 2378 series and Bovine Liver: A NIST Interlaboratory Study**; Candice Z. Ulmer[1]; John A. Bowden[1]; Christina Jones[1]; Alan Heckert[2]; Jeremy Koelmel[3]; *[1]National Institute of Standards and Technology, NIST, Hollings Marine Laboratory, Charleston, SC; [2]National Institute of Standards & Technology, NIST, Gaithersburg, MD; [3]University of Florida, Department of Chemistry, Gainesville, FL*

MP 420 **Lipid Metabolic Alterations Hallmark Pathological Processes in Human Lungs**; Lars F. Eggers[1]; Julia Müller[2]; Chakravarthy Marella[1]; Verena Scholz[1]; Henrik Watz[3, 4]; Christian Kugler[5]; Klaus F. Rabe[4, 5]; Torsten Goldmann[2, 4]; Dominik Schwudke[1, 4]; *[1]Research Center Borstel, Division of Bioanalytical Chemistry, Borstel, Germany; [2]Pathology of the University Hospital of Lübeck and the Research Center Borstel, Lübeck and Borstel, Germany; [3]Pulmonary Research Institute at LungenClinic Großhansdorf, Großhansdorf, Germany; [4]Airway Research Center North, German Center for Lung Research, Großhansdorf, Germany; [5]LungenClinic Großhansdorf, Großhansdorf, Germany*

MP 421 **Sample-per-second Shotgun Lipidomics using Acoustically-induced Electrospray Ionisation**; Martin Bachman[1]; Ian Sinclair[1]; Jonathan Wingfield[2]; Kerry

Hallbrook[1]; Sonia Houghton[1]; *[1]AstraZeneca R&D, Alderley Park, UK; [2]AstraZeneca R&D, Cambridge, UK*

MP 422 **MRM Based Phospholipid Profiling of Mouse Tissues by an Ultra-Fast Triple Quadrupole Mass Spectrometer**; Masaki Yamada[1]; Tsuyoshi Nakanishi[2]; *[1]Shimadzu Corporation, Kyoto; [2]Shimadzu Corporation, Nakagyo-ku, Japan*

MP 423 **Robust and High Throughput Lipid Profiling in Dried Blood Spot Samples Using Automated FIA MSMSAll Technique**; Kuldeep Ravivanshi[1]; Narinder Sahni[2]; Akanksha Singh[3]; Dipanakar Malakar[3]; Manoj Pillai[3]; *[1]Lipomic Healthcare Pvt. Ltd, New Delhi, India; [2]Jawaharlal Nehru University, New Delhi, India; [3]SCIEX, Gurugram, India*

MP 424 **Phospholipid Ratios in Drosophila and the Effects on the Reintroduction of SWS/NTE Mutations Back into Neurons using UPLC-HRMS/MS and SWATH**; Jeffrey Morre[1]; Claudia S. Maier[2]; Brookelyn Long[2]; Elizabeth Sunderhaus[3]; Doris Kretzschmar[3]; *[1]Oregon State University, Corvallis, OR; [2]Oregon State University, Corvallis, OR; [3]Oregon Health & Science University, Portland, OR*

MP 425 **Increase Sensitivity and Selectivity for Quantification of Phospholipids Based on Phosphate Methylation and MRM-based LC-MS/MS in Only Positive Ionization Mode**; Lili Niu[1]; Tanxi Cai[1]; Qingbo Shu[1]; Xiaojing Guo[1]; Xiang Ding[1]; Zhensheng Xie[1]; Fuquan Yang[1]; *[1]Institute of Biophysics, CAS, Beijing, China*

MP 426 **Development of a Rapid Method for Quantification of Branched Chain Fatty Acids in Phospholipids using Ion-Mobility Q-TOF Mass Spectrometry**; Peter S. Backlund[1]; Glen W. Humphrey[2]; Paul S. Blank[2]; Alfred L. Yergey[1]; Joshua Zimmerberg[2]; *[1]NICHD, NIH, Bethesda, MD; [2]Section on Membrane & Cellular Biophysics, NICHD, NIH, Bethesda, MD*

MP 427 **Lipidomic Investigation of Fenclozic Acid and Sitaxentan Treated PXB-mice using a New Scanning Quadrupole UPLC-QTof MS Acquisition Mode**; Adam King[1]; Matthew Baginski[2]; Yoshio Morikawa[2]; Robert S Plumb[1]; Ian D Wilson[1]; *[1]Imperial College, London, UK; [2]PhoenixBio USA Corp., New York, NY*

MP 428 **Untargeted RP-UPLC-QTOF- MS/MS based Shotgun Lipidomics Reveals Lipid Dynamics during High Carbohydrate or High Polyunsaturated Fatty Acid Diet**; Thekkelnaycke Rajendiran[1]; Tanu Soni[2]; Heidi Brigitte IglayReger[2]; Amy E Rothberg[2]; Charles F Burant[2]; *[1]Dept. of Pathology, University Of Michigan, Ann Arbor, MI; [2]University of Michigan Medical Center, Ann Arbor, MI*

MP 429 **Systems Biology Approach to Define the Molecular Mechanisms of Galactic Cosmic Ray induced Hepatocellular Carcinoma**; Brooke L. Barnette[1]; Shinji K. Strain[1]; Cheryl F. Lichti[1]; Yu Yongjia[1]; Robert L. Ullrich[1]; Mark R. Emmett[2]; *[1]University of Texas Medical Branch, Galveston, TX; [2]University of Texas Medical Branch, Galveston, TX*

MP 430 **Analysis of Lipids Extracted from Plant and Insect Tissues using a Chromatography Based HRMS Method with Automated Data Processing** ; Daniel Gachotte[1]; Yelena Adelfinskaya[2]; Jeffrey R Gilbert[2]; Jesse L Balcer[2]; David A Peake[3]; Lyudmila LV Sidorenko[2]; *[1]Dow AgroSciences, Indianapolis, IN; [2]Dow AgroSciences, Indianapolis, IN; [3]ThermoFisher, San Jose, CA*

MP 431 **Lipid Profiling of Six Breast Cancer Cell Lines to Understand the Mechanism of Brain Metastatic Breast Cancer**; Masoud Zabet Moghaddam[1]; Ruchika Bhawal[1]; Wenjing Peng[1]; Susan San Francisco[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

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MP 432 **Infrared Ion Spectroscopy Applied in Metabolomics and Drug Metabolism**; Jonathan Martens[1]; Giel Berden[1]; Rianne E. van Outersterp[1]; Leo A. J. Kluijtmans[2]; Udo F. Engelke[2]; Clara D. M. van Karnebeek[3, 4]; Ron A. Wevers[2]; Valerie Koppen[5]; Filip Cuyckens[5]; Jos Oomens[1, 6]; *[1]FELIX Laboratory - Radboud University, Nijmegen, Netherlands; [2]Translational Metabolic Laboratory - Radboud University Medical Center, Nijmegen, Netherlands; [3]Department of Pediatrics - University of British Columbia, Vancouver, BC, Canada, Canada; [4]Centre for Molecular Medicine - University of British Columbia, Vancouver, BC, Canada; [5]Pharmacokinetics, Dynamics & Metabolism - Janssen R&D, Beerse, Belgium; [6]van't Hoff Institute for Molecular Sciences - University of Amsterdam, Amsterdam, Netherlands*

MP 433 **Merging Targeted and Non-Targeted Metabolomics via Anion-Exchange Chromatography Coupled to High Resolution Mass Spectrometry**; Michaela Schwaiger[1]; Yasin El Abiead[1]; Evelyn Rampler[1]; Gerrit Hermann[1, 2]; Gunda Koellensperger[1]; *[1]University of Vienna, Vienna, Austria; [2]ISOtopic Solutions, Vienna, Austria*

MP 434 **Redox State Alteration at the Onset of Development in D. melanogaster**; Boryana Petrova[1]; Maiko Kitaoka[2]; Elizaveta Freinkman[1]; Iva Kronja[1]; Terry Orr-Weaver[1, 2]; *[1]Whitehead Institute, Cambridge, MA; [2]Dept. of Biology, Massachusetts Institute of Technology, Cambridge, MA*

MP 435 **Smart Data Dependent MS/MS: Toward Comprehensive MS/MS Feature Coverage in Non-Targeted Metabolomics**; Corey D Broeckling[1]; Emmy Hoyes[2]; Jeff Brown[2]; Jessica E. Prenni[1]; *[1]Colorado State University's Proteomics and Metabolomics Facility, Fort Collins, CO; [2]Waters Corporation, Wilmslow, UK*

MP 436 **Development of an Efficient Quantitative Assay for All Mevalonate Pathway Metabolites using Targeted LC-MS to Study Ovarian Cancer Metabolism**; Hamid R Baniasadi[1]; Aaron R. Goldman[1]; Hsin-Yao Tang[1]; David W Speicher[1]; *[1]Wistar Institute, Philadelphia, PA*

MP 437 **Construction of Novel Calibration-Curve-Locking Database for Metabolomic Analysis by GC/MS**; Yuki Soma[1]; Toshiyuki Yamashita[1]; Kosuke Hata[1]; Masatomo Takahashi[1]; Kuniyo Sugitate[2]; Takeshi Serino[2]; Hiromi Miyagawa[3]; Kenichi Suzuki[3]; Takatomo Kawamukai[4]; Teruhisa Shiota[4]; Kayoko Yamada[4]; Yoshihiro Izumi[1]; Takeshi Bamba[1]; *[1]Kyushu University, Fukuoka, Japan; [2]Agilent Technologies Co. Ltd, Hachioji, Japan; [3]GL Sciences Inc., Shinjuku-ku, Japan; [4]AMR Inc., Meguro-ku, Japan*

MP 438 **Comprehensive Amino Acid and DBS Analysis with a Microchip Capillary Electrophoresis-ESI Miniature Mass Spectrometry Platform in 150 Seconds**; Michael Goodwin[1]; J. Scott Mellors[1]; Erin A. Redman[1]; Glenn A. Harris[1]; Christopher Brown[1]; *[1]908 Devices Inc., Boston, MA*

MP 439 **Challenging the C1 Folate Cycle Paradigm with Probiotic Lactobacillus reuteri**; Abby J Chiang[1]; Daniel Röth[1]; Gabriel Gugiu[1]; James Versalovic[2]; Markus Kalkum[1]; *[1]City of Hope, Duarte, CA; [2]Texas Children's Hospital, Houston, TX*

MP 440 **Direct Analysis of Terpenes from Biologically Relevant Buffers using Infrared Matrix-Assisted Laser Desorption Electrospray Ionization (IR-MALDESI)**; Milad Nazari[1]; Sean R. Lund[1]; Gavin J. Williams[1]; Jon D. Williams[2]; David C. Muddiman[1]; *[1]North Carolina State University, Raleigh, NC; [2]AbbVie, North Chicago, IL*

MP 441 **Metabolomics of Biofluids from Nonhuman Primate Exposed to Ionizing Radiation**; Evan Pannkuk[1]; Evagelia C Laiakis[2]; Simon Authier[3]; Karen Wong[3]; Albert J. Fornace[1, 2]; *[1]Tumor Biology Program, Lombardi Comprehensive*

Cancer Center, Georgetown University, Washington, DC; [2]Department of Biochemistry and Molecular & Cellular Biology, Georgetown University, Washington, DC; [3]CiToxLAB North America, Laval, QC, Canada

MP 442 **Integration of Volumetric Absorptive Microsampling with a Mass Spectrometry-Based Metabolomics Workflow**; Giuseppe Paglia[1]; Chiara Volani[1, 2]; Giulia Caprioli[1]; Baldur Sigurdsson[1]; Guenter Weiss[2]; Sigurdur Smarason[1]; *[1]EURAC Research, Bolzano, Italy; [2]Medical University of Innsbruck., Innsbruck, Austria*

MP 443 **Metabolomics of Cotton Fiber**; Manoj S. Ghaste[1]; Vladimir Shulaev[1]; *[1]Department of Biological Sciences, University of North Texas, Denton, TX*

MP 444 **Combining Benzoyl Chloride Derivatization with Accurate Mass Qualitative and Quantitative Analysis to Increase Understanding of Neurological Systems**; Stefan Thibodeaux[1]; Kimberly Malesky[1]; Madeline Weber[1]; Clayton Springer[1]; Shu Li[1]; *[1]Novartis, Cambridge, MA*

MP 445 **Analysis of Non-Mevalonate (MEP) Pathway Standards and Metabolites in Cell Lysate Using a Novel LC-MS/MS Method**; Allison Fabino Carr[1]; Michael Lesslie[1]; Darshan C. Patel[2]; Victor V. Ryzhov[1]; Daniel W. Armstrong[2]; *[1]Northern Illinois University, Dekalb, IL; [2]University of Texas at Arlington, Arlington, TX*

MP 446 **Evaluation of Different Cell Harvesting and Lysis Methods for Chemical Isotope Labeling LC-MS Metabolomics**; Xinyun Gu[1]; Xian Luo[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB, Canada*

MP 447 **Metabolic Changes in Lung Tissue of Tuberculosis-Infected Mice using GC/Q-TOF**; Mª Fernanda Rey-Stolle[1]; Vineel P Reddy[2]; Santiago Angulo[1]; Adrie JC Steyn[2, 3, 4]; Sofia Nieto[5]; Nathan Eno[5]; Coral Barbas[1]; *[1]CEMBIO (Centro de Metabolómica y Bioanálisis), Facultad de Farmacia, Universidad CEU San Pablo, Madrid, Spain; [2]Department of Microbiology, University of Alabama at Birmingham, Birmingham, AL; [3]KRITH (KwaZulu-Natal Research Institute for TB and HIV), Durban, South Africa; [4]UAB Center for Free Radical Biology, University of Alabama at Birmingham, Birmingham, AL; [5]Agilent Technologies Inc., Santa Clara, CA*

MP 448 **Metabolomic Approach for Carotenoids Analysis of Chrysanthemum Flower by Liquid Chromatograph Tandem Mass Spectrometry**; Junichi Masuda[1]; Satoshi Yamaki[2]; Yoshihiro Hayakawa[2]; Masaru Furuta[2]; Yuji Sawada[3]; Mami Okamoto[3]; Muneo Sato[3]; Masami Y. Hirai[3]; *[1]Shimadzu Corporation, Hadano-city, Japan; [2]Shimadzu Corporation, Kyoto, Japan; [3]RIKEN Center for Sustainable Resource Science, Yokohama, Kanagawa*

MP 449 **Quantitative and Qualitative Metabolic Flux Analysis via a Novel Data Independent Acquisition Mode 'SONAR' using High Resolution Mass Spectrometry**; Paul Rainville[1]; Chris Beecher[2]; Jose Castro-Perez[3]; James Langridge[4]; David Heywood[4]; *[1]Waters, Milford, MA; [2]IROA Technologies, Gainesville, Florida; [3]Waters Corp, Milford, MA; [4]Waters Corp., Wilmslow, UK*

MP 450 **Metabolomic Analysis of Microbiome Transplantation in Mice**; Jason Winnike[1]; David Kirchner[1]; Kevin Knagge[1]; Brian Bennett[2]; *[1]David H. Murdock Research Institute, Kannapolis, NC; [2]United States Department of Agriculture Agricultural Research Service, Davis, CA*

MP 451 **Metabolomic Interrogation of the Mechanisms of Radiation-Induced Lung Injury**; Jenna Alloush[1]; Jace W. Jones[2]; Claire Louise Carter[2]; Isabel L Jackson[3]; Zeljko Vujaskovic[3]; Maureen A Kane[2]; *[1], Baltimore, MD; [2]University of Maryland School of Pharmacy, Baltimore, MD; [3]University of Maryland School of Medicine, Baltimore, MD*

MP 452 **Application of Isotopically Nonstationary Flux Analysis for Nucleotides Metabolism Studies in Human Cells**; Fedor Kryuchkov; *University of Bergen, Bergen, Norway*

MP 453 **Comprehensive Analysis of Hydrophilic Metabolites by Coupling Ion Chromatography and PFPP-based Liquid Chromatography Methods to High Resolution Mass Spectrometry**; Yoshihiro Izumi[1]; Takahiro Suzuki[2]; Masatomo Takahashi[1]; Kohta Nakatani[1]; Kiyotaka Oshikawa[1]; Motokazu Kimura[2]; Takahara Kentaro[2]; Masaki Matsumoto[1]; Takeshi Bamba[1]; *[1]Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan; [2]Thermo Fisher Scientific Japan, Tokyo, Japan*

MP 454 **Targeted LC-MS/MS Based Metabolomics Revealing Staphylococcus aureus Metabolic Reprograming, from Planktonic to Biofilm**; Chen Wang[1]; Jiangjiang Zhu[1]; *[1]Miami University, Oxford, Ohio*

MP 455 **Mice Fecal Metabolomics by LC-MS/MS: Comparison between Young Mice and Old Mice**; Takanari Hattori[1, 2]; Shuichi Kawana[1]; Yoshihiro Hayakawa[1]; Eiichiro Fukusaki[3]; Mitsuharu Matsumoto[4]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Osaka University Shimadzu Analytical Innovation Research Laboratory, Suita, Japan; [3]Osaka University, Suita, Japan; [4]Kyodo Milk Industry Co. Ltd., Nishitama, Japan*

MP 456 **Steroid and Tricarboxylic Acid Cycle Isobar Separation and Quantitation using Ion Mobility-QTOF and LC/MS/MS**; Sumankalai Ramachandran[1]; Minas Sakellakis[1]; Zahi Mitri[2]; Niki Millward[3]; Sriram Shanmuga Velandy[3]; Pratip Bhattacharya[3]; David Piwnica-Worms[3]; Christopher Logothetis[1]; Mark Titus[1]; *[1]Koch Center, MD Anderson Cancer Center, Houston, TX; [2]Oregon Health & Science University, Portland, OR; [3]Cancer Systems Imaging, MD Anderson Cancer Center, Houston, TX*

MP 457 **High-throughput Analysis of Xenobiotics by Automated Electrochemistry/Mass Spectrometry**; Simon Gereon Scheeren[1]; Uwe Karst[1]; *[1]University of Münster, Institute of Inorganic and Analytical Chemistry, Münster*

MP 458 **Targeted and Untargeted Mass Spectrometry for Identification of Metabolomic Changes Associated with Chronic Defeat Stress in Mice**; Constance A. Sobsey[1]; Jun Han[1]; Michael J. Meaney[2, 3, 4]; Christoph H. Borchers[1, 3, 5]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Dept. of Oncology, Segal Cancer Centre, Jewish General Hospital, McGill University, Montreal, QC, Canada; [3]Dept. of Oncology, McGill University, Montreal, QC, Canada; [4]Depts. of Psychiatry and Neurology and Neurosurgery, McGill University, Montreal, QC, Canada; [5]Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

MP 459 **Development of More Reproducible and Sensitive Polar Metabolomics Methods**; Hardik Shah[1]; Steven M. Fischer[2]; Justin R. Cross[1]; *[1]Donald B. and Catherine C. Marron Cancer Metabolism Center at Memorial Sloan Kettering Cancer Center, New York, NY; [2]Agilent Technologies, Santa Clara, CA*

MP 460 **Same Sample Targeted and Untargeted Fecal Mass Spectrometry for Molecule - Microbiome Wide Association Studies**; Alexey V. Melnik[1]; Ricardo Da Silva[1]; Embriette R Hyde[2]; Fernando Vargas[1]; Amina Bouslimani[1]; Ivan Protsyuk[3]; Alan Jarmusch[1]; Alexander Aksenov[1]; Anupriya Tripathi[1, 2, 4]; Theodore Alexandrov[1, 3, 5]; Rob Knight[2, 4]; Pieter C. Dorrestein[1, 2]; *[1]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; [2]Department of Pediatrics, University of California San Diego, La Jolla, CA; [3]EMBL, Heidelberg, Heidelberg; [4]Center for Microbiome Innovation, University of California San Diego, La Jolla, CA; [5]Department of Computer Science and Engineering, University of California San Diego, La Jolla, CA*

MP 461 **Identification of Metabolite Markers of Mn2+ Accumulation in Deinococcus radiodurans by Liquid Chromatography Mass Spectrometry**; Jingyueh Jeng; *Chia Nan Univ of Pharmacy & Science , Tainan , Asia*

MP 462 **Semi-targeted Metabolomics of Oxylipins**; Jeffrey F. Kuhn[1]; Fred Bjorn Lih[1]; Matthew Edin[1]; Darryl Zeldin[1]; Leesa J Deterding[1]; *[1]NIEHS\NIH\DHHS, Research Triangle Park, NC*

MP 463 **LC-MS Metabolomic Serum Signatures Indicate Changes in Protein and Fatty Acid Metabolism Precede Retained Placenta in Dairy Cows**; Fereshteh Zandkarimi[1]; Gerd Bobe[2, 3]; Claudia S. Maier[1, 3]; *[1]Chemistry Department, Oregon State University, Corvallis, OR; [2]Department of Animal and Rangeland Sciences, Corvallis, OR; [3]Linus Pauling Institute, Oregon State University, Corvallis, OR*

METABOLOMICS: SAMPLE PREPARATION
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MP 464 **Coupling Solid Phase Microextraction to Complementary Separation Platforms for Metabotyping of E. coli Metabolome in Response to Natural Antibacterial Agents**; Fatemeh Mousavi[1]; Emanuela Gionfriddo[2]; Eduardo Carasek[3]; Erica A Souza-Silva[4]; Janusz Pawliszyn[2]; *[1]Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON, Canada; [2]University of Waterloo, Waterloo, Ontario; [3]Department of Chemistry, Federal University of Santa Catarina, Florianópolis, Brazil; [4]Universidade Federal do Rio Grande do Sul, Porto Alegre, Brazil*

MP 465 **An Approach for Metabolomics Survey of the Extracellular Vesicles in Esophageal Carcinoma Serum**; Yan Ren[1]; Ju Wang[1]; Jin Zi[1]; Liang Lin[1]; Siqi Liu[1]; *[1]BGI-Shenzhen, Shenzhen, China*

MP 466 **Automated Sample Preparation for GC/MS and LC/MS-based Metabolomics: Analysis of Contamination Sources**; Emily Davidson[1]; Sarah-Marie A Lyons[1]; Corey D. Broeckling[1]; Jessica E. Prenni[1]; *[1]Proteomics and Metabolomics Facility; Colorado State University, Fort Collins, CO*

MP 467 **A LC-MS Metabolomics Method Enabling Rapid Sample Preparation and Analysis of Polar and Unstable Metabolic Intermediates**; Tony Karlsborn[1]; Magesh Muthu[1]; Anders Nordström[1]; *[1]Department of Molecular Biology, Umeå University, Umeå, Sweden*

MP 468 **Assessment of Rapid Heat Treatment for Pre-Analytical Stabilization of the Lipidome**; Christina M Jones[1]; Jeremy P Koelmel[2]; Tracey B Schock[1]; Candice Z. Ulmer[1]; John A. Bowden[1]; *[1]National Institute of Standards and Technology, NIST, Hollings Marine Laboratory, Charleston, SC; [2]University of Florida, Department of Chemistry, Gainesville, FL*

MP 469 **Method Development for the Metabolomic Profile of Cyanobacteria with Altered Circadian Rhythms**; Berkley Ellis[1]; R. L. Gant-Branum[2]; Chi Zao[3]; Yao Zu[3]; Carl H Johnson[2]; John A. McLean[2]; *[1], Nashville, TN; [2]Vanderbilt University, Nashville, TN; [3]Vanderbilt University, Nashville, TN*

MP 470 **Untargeted Metabolomic and Lipidomic Characterization of Brain Tissue using Solid Phase Microextraction**; Ezel Boyaci[1]; Nathaly Reyes-Garcés[1]; German A Gómez-Ríos[1]; Barbara Bojko[1, 2]; Dajana Vuckovic[3]; Janusz Pawliszyn[1]; *[1]University of Waterloo, Waterloo, ON, Canada; [2]Nicolaus Copernicus University in Torun, Bydgoszcz, Poland; [3]Concordia University, Montreal, QC, Canada*

MP 471 **Automation of Sample Preparation Procedure for Hydrophilic Metabolomic and Lipidomic Analysis using a Robotic Platform**; Yuki Soma[1]; Toshiyuki Yamashita[1]; Masatomo Takahashi[1]; Kuniyo Sugitate[2]; Takeshi Serino[2]; Hiromi Miyagawa[3]; Kenichi Suzuki[3]; Takatomo Kawamukai[4]; Teruhisa Shiota[4]; Kayoko Yamada[4]; Yoshihiro Izumi[1]; Takeshi Bamba[1]; *[1]Kyushu University, Fukuoka, Japan; [2]Agilent Technologies Co. Ltd, Hachioji, Japan; [3]GL Sciences Inc., Shinjuku-ku, Japan; [4]AMR Inc., Meguro-ku, Japan*

MP 472 **Improving Metabolite Extraction in Metabolomics with Crosslinkers**; Kevin Y Cho[1]; Liz Llufrio[1]; Xiangfeng Niu[1]; Gary J. Patti[1]; *[1]Washington University School of Medicine, St. Louis, MO*

MP 473 **Extraction and Quantitation of NAD(P)(H)**; Wenyun Lu[1]; Li Chen[1]; Sheng Hui[1]; Joshua D Rabinowitz[1]; *[1]Princeton Universitry, Princeton, NJ*

MP 474 **Evaluation of an Automated LC-MS/MS System for Analyzing Hydrophilic Blood Metabolites**; Shin Nishiumi[1]; Keisuke Shima[2]; Hidekazu Saiki[2]; Takeshi Azuma[1]; Masaru Yoshida[1, 3]; *[1]Kobe University Graduate School of Medicine, Kobe, Japan; [2]Shimadzu Corporation, Kyoto, Japan; [3]AMED, Kobe, Japan*

METABOLOMICS: TARGETED AND QUANTITATIVE ANALYSIS I
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MP 475 **Liquid Chromatography Tandem Mass Spectrometric Analysis of Bile Acids in Biological Samples**; Jaeman Byun[1]; Anna V. Mathew[1]; Adil Jadoon[1]; Subramaniam Pennathur[1]; *[1]University of Michigan, Ann Arbor, MI*

MP 476 **N-omics: Metabolomics for N-containing Metabolites**; Ryo Nakabayashi[1]; Kei Hashimoto[1]; Tetsuya Mori[1]; Kiminori Toyooka[1]; Kazuki Saito[1, 2]; *[1]RIKEN Center for Sustainable Resource Science, Yokohama, Kanagawa; [2]Chiba Univevrsity, Chiba, Japan*

MP 477 **Multivariate Approach to Optimize a Novel Diagnostic One-Pot Derivatization Kit for Biomarkers of BTEX**; Yehia Baghdady[1]; Kevin A. Schug[1]; *[1]The University of Texas at Arlington, Arlington, TX*

MP 478 **Identification and Quantitation of Long Chain Fatty Acids byTargeted Metabolomics**; Chandra Shekar R Ambati[1]; Nagireddy Putluri[1]; Arun Sreekumar[1]; Vivekananda Shetty[1]; *[1]Baylor College of Medicine, Houston, TX*

MP 479 **Human Plasma Targeted-Metabolomics Using an Amine Derivatization Reagent**; Kazutaka Shimbo; *Ajinomoto CO., INC, Kawasaki-Shi, Kanagawa*

MP 480 **Using Metabolomics to Characterize Marine Organic Matter Cycling by Microbes**; Melissa C. Kido Soule[1]; Krista Longnecker[1]; Cara L. Fiore[2]; Jamie W. Becker[3]; Rogier Braakman[3]; Keven Dooley[3]; Allison Coe[3]; Sallie W. Chisholm[3]; Elizabeth B. Kujawinski[1]; *[1]Woods Hole Oceanographic Ins, Woods Hole, MA; [2]Appalachian State University, Boone, North Carolina; [3]Massachusetts Institute of Technology, Cambridge, MA*

MP 481 **An Isotope-Labeling Chemical Derivatization - UPLC/MRM-MS Method for Accurate Quantitation and Stability Testing of Carnitines in Dried Blood Spots**; Jun Han[1]; Rehan Higgins[1]; Juncong Yang[1]; Karen Lin[1]; Kieran Atkinson[1]; Christoph H. Borchers[1, 2]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

MP 482 **A Targeted LC-MS/MS Method for Separation and Quantification of Numerous Vitamin D Metabolites including 1α,25(OH)2D, 3-EPI-25OHD3, and 25OHD3**; Brian C Defelice[1, 2]; Oliver Fiehn[1, 2]; *[1]West Coast Metabolomics Center, Davis, CA; [2]University of California, Davis, Davis, CA*

MP 483 **Collaborative Cross Founder Mouse Strain Profiling via Targeted Metabolomic Library**; Dorothy Ahlf Wheatcraft[1]; Rob Wilpan[2]; Ruth Saxl[2]; *[1]Jackson Laboratory, Bar Harbor, ME; [2]The Jackson Laboratory, Bar Harbor, ME*

MP 484 **Evaluation of High Speed, High Resolution Data Independent Acquisition for Simultaneous Identification and Quantitative Metabolomic Flux Analysis**; Loren Olson[1]; Emile Plise[2]; Baljit Ubhi[1]; *[1]SCIEX, Redwood City, CA; [2]Genentech, Inc, South San Francisco, CA*

MP 485 **Validation and Characterization of the iROA Standard Library using High Resolution Mass Spectrometry**; Vilinh Tran[1]; Ken Liu[1]; Dean P Jones[1]; *[1]Emory School of Medicine, Atlanta, GA*

MP 486 **Detection and Quantitation of Sugar Phosphate Metabolite Markers in Femto Molar Concentration using 6500+ QTRAP LCMS/MS System**; Manoj Pillai[1]; Dipankar Malakar[1]; Faraz Rashid[1]; *[1]ABSCIEX, Gurgaon, Haryana*

MP 487 **Separation, Identification and Quantification of Peptidoglycan Fragments by Zwitterionic Hydrophilic Interaction Chromatography and Capillary Electrophoresis Coupled to Mass Spectrometry**; Madeleine Boulanger[1, 2]; Alice Raymackers[2]; Cédric Delvaux[1]; Johann Far[1]; Loïc Quinton[1]; Edwin De Pauw[1]; Bernard Joris[2]; *[1]Mass Spectrometry Laboratory, Liège, Belgium; [2]Center for Protein Engineering, Liège, Belgium*

MP 488 **Quantitative Profiling of Central Carbon Metabolites by Liquid Chromatography-Mass Spectrometry**; Yan-Ping Lin[1]; Benjamin A. Garcia[1]; *[1]University of Pennsylvania, Philadelphia, PA*

MP 489 **Nano LC-MS/MS Method Development for the Analysis of Steroids in Whale Blubber for Reproductive Fitness and Stress Assessments**; Ruchika Bhawal[1]; Mary Hayden[1]; John Escobedo[1]; Clinton Harmon[1]; David Klein[1]; Susan San Francisco[1]; Masoud Zabet Moghaddam[1]; Celine Godard-Codding[1]; *[1]Texas Tech University, Lubbock, TX*

MP 490 **Targeting the Long Game: Assessing Longitudinal Precision and Bias of Two Targeted Metabolomics Platforms in the Context of Clinical Metabolomics**; J. Will Thompson [1]; Lisa St. John-Williams[1]; M. Arthur Moseley[1]; *[1]Duke University School of Medicine, Durham , NC*

MP 491 **Quantification of Amino Acids using Isotopic Ratio Outlier Analysis (IROA) and LC-MS/MS**; Vanessa Y. Rubio[1]; Chris Beecher[2, 3]; Richard A. Yost[1]; Timothy J. Garrett[4]; *[1]University of Florida, Department of Chemistry, Gainesville, FL; [2]IROA Technologies, Gainesville, Florida; [3]University of Florida, Gainesville, FL; [4]University of Florida, Department of Immunology, Pathology, and Laboratory Medicine, Gainesville, FL*

MP 492 **Quantitative LC-MS/MS Analysis of 100 Intracellular Metabolites of Clostridium autoethanogenumusing Multiple Uniformly 13C-labelled Internal Standards**; Laudina Safo[1]; Alex Grosse-Honebrink[2]; Salah Abdelrazig[2]; Bart Pander[2]; Anne M. Henstra[2]; Rupert Norman[2]; Thomas Millat[2]; Neil R Thomas[2]; Klaus Winzer[2]; Dong-Hyun kim[2]; Nigel Minton[2]; David A. Barrett[2]; *[1]University of Nottingham, nottingham; [2]University of Nottingham, School of Pharmacy, Nottingham, UK*

MP 493 **Determination of TCA Metabolites by Ion Chromatography HR/AM Mass Spectrometry**; Terri T Christison[1]; Shen Hu[2]; Ralf Tautenhahn[1]; Reiko Kiyonami[1]; Jeffrey S Rohrer[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]University of California, Los Angeles, Los Angeles, CA*

MP 494 **Targeted Metabolomics using LC-QqQLIT, Data-Dependent Acquisition, and Scheduled SRM**; Michel Wagner[1]; Marc Turgeon[1]; George Poulogiannis[1]; *[1]The Institute of Cancer Research, London*

MP 495 **Solvent-compensation liquid Chromatography System Coupled with Multiple Detectors in the Analysis of Metabolites Related to the Quality of Tea**; Che-I Liao[1]; Zong-Yi Wu[1]; Kuo-Lung Ku[1]; *[1]National Chiayi University, Chiayi City, Taiwan*

METABOLOMICS: UNTARGETED METABOLITE PROFILING I
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MP 496 **Comparative Metabolic Profiling of Metastatic and Primary Melanoma Cell Lines**; Zhihao Yu[1]; Ming Huang[2]; Brian Clowers[1]; *[1]Washington State University, Pullman, WA; [2]University of California, Riverside, Riverside, CA*

MP 497 **Separating Metabolites Basing on Their Structural Properties: A Metabolomics Case Study, and Potential Path to Molecular Structure Digitization**; Gang Xing[1]; Michelle F. Clasquin[1]; Meihua Tu[1]; Thomas V. Magee[1]; *[1]Pfizer, Cambridge, MA*

MP 498 **Molecular Biogeography of the Heart Identifies Determinants of Chagas Disease Progression**; Laura-Isobel McCall[1]; James T. Morton[1]; Jair Lage de Siqueira-Neto[1]; Rob Knight[1]; Pieter C. Dorrestein[1]; James H. McKerrow[1]; *[1]University of California San Diego, San Diego, CA*

MP 499 **Multiplatform Metabolomics Reveals Predictive Prostate Cancer Recurrence Phenotypes Following Radical Prostatectomy**; Chaevien S. Clendinen[1]; David A. Gaul[1]; Rebecca S. Arnold[2]; Arthur S. Edison[3]; John A. Petros[2, 4]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]Emory University, Atlanta, Georgia; [3]University of Georgia, Athens, GA; [4]Atlanta VA Medical Center, Atlanta, GA*

MP 500 **Metabolomic Signatures in Urine from Renal Cell Carcinoma Patients**; David A. Gaul[1]; Chaevien S. Clendinen[1]; Rebecca S. Arnold[2]; John A. Petros[2]; Facundo M. Fernandez[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]Emory University, Atlanta, GA*

MP 501 **Proteomics and Metabolomics Profiles of Endothelial Cells under High and low Shear Stress: Understanding the Atherosclerosis Onset at Molecular Level**; Gabriela Venturini Silva[1]; Rafael Dariolli[1]; Kallyandra Padilha[1]; Pamella Araujo Malagrino[1]; Tamiris Gois[1]; Valdemir Melechco Carvalho[2]; Jessica Silva Salgueiro[2]; Karina Morais Cardozo[2]; Jose Eduardo Krieger[1]; Alexandre Costa Pereira[1]; *[1]Incor - FMUSP, Sao Paulo, Brazil; [2]Fleury Group, Sao Paulo, Brazil*

MP 502 **Curatr: A Browser Based Platform for Building High Quality Spectral Libraries**; Andrew Palmer[1]; Prasad Phapale[1]; Dominik Fay[1]; Theodore Alexandrov[1, 2]; *[1]EMBL, Heidelberg, Baden-Wuerttemberg; [2]Skaggs School of Pharmacy, University of California San Diego, La Jolla, CA*

MP 503 **A Pilot Multiplatform Metabolomic Fingerprinting Study of Plasma Metabolic Alterations in Breast Cancer**; Mónica Cala[1]; Julian Aldana[1]; Jessica Medina[2]; Julian Sanchez[3]; Jose Guio[3]; Julien Wist[2]; Roland Meesters[1]; *[1]Universidad de los Andes, Bogotá, D.C., Colombia; [2]Universidad del Valle, Cali, Colombia; [3]Liga contra el Cancer Seccional Bogotá, Bogotá, D.C., Colombia*

MP 504 **Intra- and Inter-Lab LC-MS Data Comparison for Studying Portability of a Metabolite Library for Rapid Metabolite Identification in Metabolomics**; Shuang Zhao[1]; Xian Luo[1]; Ulrike Schweiger Hufnagel[2]; Aiko Barsch[2]; Liang Li[1]; *[1]University of Alberta, Edmonton, Alberta; [2]Bruker Daltonik GmbH, Bremen, Germany*

MP 505 **Metabolomic Profile of Tambaqui Fish (Colossoma macropomum, Cuvier 1818) under Hypoxia**; Clécio Fernando Klitzke[1]; Marcos N. Eberlin[2]; Adalberto L Val[1]; *[1]Laboratory of Ecophysiology and Molecular Evolution, Brazilian National Institute for Research of the Amazon, Manaus, Brazil; [2]ThoMSon Mass Spectrometry Laboratory, Institute of Chemistry, University of Campinas, Campinas, Brazil*

MP 506 **Development of Chemical Isotope Labeling Liquid Chromatography Mass Spectrometry for Profiling the Carbonyl Submetabolome**; Shuang Zhao[1]; Margot Dawe[1]; Kevin Guo[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB, Canada, Canada*

MP 507 **Changes in Plasma Metabolites of Patients with Atrial Fibrillation**; Youngae Jung[1, 2]; Geum-Sook Hwang[1, 3]; *[1]Western Seoul Center, Korea Basic Science Institute, Seoul, South Korea; [2]Department of Life Science, Ewha Womans University, Seoul, South Korea; [3]Department of Chemistry and Nano Science, Ewha Womans University, Seoul, South Korea*

MP 508 **Profiling of Polyphenols in Fruits and Vegetables by UPLC-(ESI)-QToF-MS with UNIFI-based Data Processing**; Dasharath Pandurang Oulkar[1]; Zareen Khan[1]; Kaushik Banerjee[1]; *[1]National Referral Laboratory, ICAR-National Research Centre for Grapes, Manjri Farm, Pune, India*

MP 509 **Determining Impacts of a Natural Product Biosynthetic Pathway on Streptomyces Metabolomes by Isotopic Ratio Outlier Analysis (IROA) Global Metabolomics**; Amy L Lane[1]; Elle D James[1]; Felice A de Jong[2]; Chris Beecher[3]; *[1]University of North Florida, Jacksonville, FL; [2]IROA Technologies LLC, Bolton, MA; [3]University of Florida, Gainesville, FL*

MP 510 **MALDI-MSI Allows Identification and Semi-Quantification of Endogenous Cardenolides Associated with Glioblastoma Cells Death under ZIKV Infection**; Estela de Oliveira Lima[1]; Tatiane Melina Guerreiro[1]; Carlos Fernando O. R. Melo[1]; Diogo Noin de Oliveira[1]; Daisy Machado[2]; Marcelo Lancellotti[2]; Rodrigo Ramos Catharino[1]; *[1]Innovare Biomarkers Laboratory, Campinas, Brazil; [2]Laboratory of Biotechnology, Campinas, Brazil*

MP 511 **Global Metabolomic Investigation of Tissues from Melanoma Patients with HRMS Using a Yeast Standard for Isotopic Ratio Outlier Analysis (IROA)**; Taylor M. Domenick[1]; Chris Beecher[2, 3]; Louis Searcy[1]; Peter A. Kanetsky[4]; Richard A. Yost[1]; Nicholas Taylor[5]; Timothy J. Garrett[6]; *[1]University of Florida, Department of Chemistry, Gainesville, FL; [2]IROA Technologies, Gainesville, Florida; [3]University of Florida, Gainesville, FL; [4]H. Lee Moffitt Cancer Center and Research Institute, Tampa, FL; [5]Texas A&M University, College Station, TX; [6]University of Florida, Department of Immunology, Pathology, and Laboratory Medicine, Gainesville, FL*

MP 512 **Metabolomic Studies of Pyrazinamide in Mycobacterium Tuberculosis Using an Ion-pairing Reverse Phase Q-TOF LC/MS Approach**; Yuqin Dai[1]; Travis E Hartman[2]; Steve M Fischer[1]; Kyu Y Rhee[2, 3]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]Division of Infectious Diseases, Department of Medicine, Weill Cornell Medical College, New York, NY; [3]Department of Microbiology and Immunology, Weill Cornell Medical College, New York, NY*

MP 513 **Global Plasma Metabolic Profiles in Term and Preterm Birth**; Brittany Lee-McMullen[1]; Kevin Contrepois[1]; Martin Angst[1]; Brice Gaudillere[1]; Stephen Quake[1]; David A. Relman[1]; Gary M. Shaw[1]; David K. Stevenson[1]; Mike Snyder[1]; *[1]Stanford University, Stanford, CA*

MP 514 **Metabolic Effects in Atorvastatin-Treated Liver Cells**; Gabriela Venturini[1]; Kallyandra Padilha[1]; Rafael Dariolli[1]; Pamella Araujo Malagrino[1]; Jose Eduardo Krieger[1]; Alexandre Costa Pereira[1]; *[1]Heart Institute, Sao Paulo, SP*

MP 515 **Untargeted Investigation of Non-alcoholic Fatty Liver Disease Using Effective Multiplatform GC-MS Instrumentation**; David Alonso[1]; Xiang Zhang[2]; Joe Binkley[3]; *[1]LECO Corporation, St. Joseph, MI; [2]University of Louisville, Louisville, KY; [3]LECO Corporation, St Joseph, MI*

MP 516 **The Effect of Sleep and Circadian Disruption on the Human Metabolome**; Fernando Vargas[1]; Christopher Depner[2]; Antonio González Peña[3]; Kenneth Wright[2]; Rob Knight[3]; Pieter C. Dorrestein[1]; *[1]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; [2]University of Colorado, Boulder, CO; [3]Department of Pediatrics, University of California San Diego, San Diego, CA*

MP 517 **Untargeted Metabolomics Reveals Novel Metabolites within the Coastal and Open Ocean**; Elizabeth Kujawinski[1]; Winifred Johnson[1]; Melissa C. Kido Soule[1]; Krista Longnecker[1]; *[1]Woods Hole Oceanographic Inst., Woods Hole, MA*

MP 518 **Utilizing an Untargeted Ion Mobility-Mass Spectrometry Method to Profile Changes in the Gut Metabolome**; James Poland[1]; Alexandra C Schrimpe-Rutledge[1]; Charles Robb Flynn[1]; John A. McLean[1]; *[1]Vanderbilt University, Nashville, TN*

MP 519 **Metabolic Reprogramming by ETHE1, a Mitochondrial Persulfide Dioxygenase**; Changyuan Lu[1]; Joshua Benjamin Zuk[1]; Steven Gross[1]; *[1]Weill Medical College of Cornell, New York, NY*

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MP 521 **An HS-MRM Assay for Quantification of Host Cell Proteins in Therapeutic Monoclonal Antibodies**; Catalin Doneanu[1]; Jing Fang[2]; Yun Alelyunas[2]; Ying Qing Yu[2]; Mark Wrona[2]; Weibin Chen[2]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Milford, MA*

MP 522 **An Open-Source Tool for the Creation of Multiplexed, Targeted Proteomic Instrument Methods Utilizing Isobaric Labels**; Christopher Rose[1, 2]; Brian K Erickson[2]; Steven Gygi[2]; Donald Kirkpatrick[1]; *[1]Genentech, Inc., South San Francisco, CA; [2]Harvard Medical School, Boston, MA*

MP 523 **Building ProteomeTools Based on a Complete Synthetic Human Proteome**; Daniel P. Zolg[1]; Mathias Wilhelm[1]; Karten Schnatbaum[2]; Johannes Zerweck[2]; Tobias Knaute[2]; Bernard Delanghe[3]; Hans-Christian Ehrlich[4]; Peng Yu[1]; Siegfried Gessulat[1, 4]; Maximilian Weiniger[1]; Tobias K Schmidt[1]; Patroklos Samaras[1]; Karl Kramer[1]; Judith Schlegl[5]; Holger Wenschuh[2]; Thomas Moehring[3]; Stephan Aiche[4]; Andreas F. Huhmer[6]; Ulf Reimer[2]; Bernhard Kuster[1, 7]; *[1]Technical University of Munich, Freising, Germany; [2]JPT Peptide Technologies GmbH, Berlin, Germany; [3]Thermo Fisher Scientific, Bremen, Germany; [4]SAP SE, Potsdam, Germany; [5]SAP SE, Walldorf, Germany; [6]ThermoFisher, San Jose, CA; [7]Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany*

MP 524 **A Highly Effective Workflow for the Targeted Detection of Peptides in Complex Biological Sample Matrices from Discovery to Quantitation**; David Sarracino[1]; Susan E Abbatiello[1]; Scott Peterman[1]; Amol Prakash[2]; Shen Luan[1]; Claudia Martins[3]; Mary Blackburn[3]; *[1]Thermo Scientific, Cambridge, MA; [2]Optys Technologies, Boston, MA; [3]Thermo Fisher Scientific, San Jose, CA*

MP 525 **DesigningTargeted Detection of Peptides in Complex Matrices combining the MIDAS™ Workflow with the Skyline Software**; Jenny Albanese[1]; Christie Hunter[2]; Kaipo Tamura[3]; Brendan MacLean[4]; *[1]Jenny Albanese, Redwood City, CA; [2]Christie L. Hunter, Redwood City, CA; [3]Kaipo Tamura, Seattle, WA 98105; [4]Brendan, Seattle, WA*

MP 526 **Optimized Peptide Retention Time Standards for Targeted Proteomics**; Lawrence Eckler[1]; Karsten Schnatbaum[1]; Daniel Zlog[2]; Tobias Knaute[1]; Mathias Wilhelm[3]; Bernhard Kuster[4]; *[1]JPT Peptide Technologies, Berlin; [2]Technical University of Munich, Freising, Germany; [3]Center for Integrated Protein Science Munich, Freising, Germany; [4]Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany*

MP 527 **Proteomic Connectivity Maps of Chromatin and Phosphosignaling: Community Resources for Drug Discovery and Functional Genomics**; Lev Litichevskiy[1]; Adam Officer[1]; Amanda Creech[1]; Shawn Egri[1]; Malvina Papanastasiou[1]; Ryan Peckner[1]; Xiaodong Lu[1]; Daniel Lam[1]; Desiree Davison[1]; Tak Ko[2]; Vagisha Sharma[3]; Fatema Abdurrob[2]; Jennie Z. Young[2]; David L. Lahr[1]; Alison Mungenast[2]; Jarrett Egertson[3]; Steven A. Carr[1]; Michael J MacCoss[3]; Li-Huei Tsai[2]; Jacob D. Jaffe[1]; *[1]The Broad Institute, Cambridge, MA; [2]Massachusetts Institute of Technology, Cambridge, MA; [3]University of Washington, Seattle, WA*

MP 528 **Scout-MRM Simplifies Targeted Assay Development from Public Proteomic Dataset: A Yeast Proteome Case Study**; Lény Garcia[1]; Romain Carriere[1]; Eric Testet[2]; Pathy Laquel[3]; François Doignon[3]; Yves LeBlanc[4]; Ayciriex Sophie[1]; Jérôme Lemoine[5]; *[1]Institut des Sciences Analytiques, Université de Lyon, Université Lyon 1, Ens de Lyon, CNRS, Lyon, France; [2]Institut Polytechnique de Bordeaux, Bordeaux, France; [3]Université de Bordeaux, Bordeaux, France; [4]SCIEX, Concord, ON, Canada, ON, Canada; [5]Université de Lyon, Villeurbanne*

MP 529 **Towards Accurate Multiplexed Protein Mass Spectrometry for the Masses**; Martin Wühr[1]; Graeme McAlister[2]; Matthew Sonnett[1]; *[1]Princeton University, Princeton, NJ; [2]ThermoFisher, San Jose, CA*

MP 530 **Trends in Disulfide Bond Formation in Cysteine Containing Small Peptides**; Michael D. Browne[1]; LeRoi de-Souza[1]; Ekram Hossain[1]; Jianhua Ren[1]; *[1]University of the Pacific, Stockton, CA*

MP 531 **Selective Capture and Analysis of Azido Compounds Using aPropargyl-based Cleavable Linker**; Michael GJ Doyle[1]; Baylie Gigolyk[1]; Michelle Mclellan[1]; Vinith Yathindranath[1]; Edward D Bodnar[2]; Helene Perreault[3]; *[1]University of Manitoba, Winnipeg, MB; [2]Agilent Technologies, Inc., Wilmington, DE; [3]University of Manitoba, Winnipeg, MB*

MP 532 **Bioanalytical Method Development for Therapeutic Peptides: Strategies for Overcoming LC/MS/MS-based Assay Hurdles**; Moucun Yuan[1]; Eric Ma[1]; William Mylott[1]; Rand Jenkins[1]; *[1]PPD Laboratories, Richmond, VA*

MP 533 **Targeted Neuropeptidomics: Parallel Reaction Monitoring or Data-Independent Acquisition for the Analysis of Neuropeptides using High-Resolution Mass Spectrometry**; Mouna Saidi[1]; Soufiane Kamali[1]; Francis Beaudry[1]; *[1]Université de Montréal, St-Hyacinthe, QC, Canada*

MP 534 **Implementation of Capillary Zone Electrophoresis Methods in Quantitative Proteomics**; Simion Kreimer[1]; Benjamin C Orsburn[2]; Robert N. O'mealy[1]; Robert N. Cole[1]; *[1]Mass Spectrometry and Proteomics Facility, Johns Hopkins School of Medicine, Baltimore, Maryland; [2]Thermo Fisher Scientific, Baltimore, Maryland*

MP 535 **Using Electrokinetic Injection to Increase Throughput and Improve Sensitivity in the Detection of Basic Neuropeptides by Capillary Electrospray Ionisation (CESI)**; Stephen J. Lock[1]; Jim Thorn[1]; Edna Betgovargez[2]; Bryan Fonslow[2]; *[1]SCIEX, Warrington, UK; [2]Sciex, Brea, CA*

MP 536 **A Standard Assessment of the Extracellular Vesicles' Purification Methods by Targeted Mass Spectrometry**; Tingting Wang[1, 2]; Kyle W Anderson[1, 2]; Illarion V. Turko[1, 2]; *[1]NIST, Gaithersburg, MD; [2]Institute for Bioscience and Biotechnology, Rockville, MD*

MP 537 **A Carrier-Assisted Targeted Mass Spectrometry Approach for Proteomics Analysis of Single Cells** ; Tujin Shi[1]; Matthew J. Gaffrey[1]; Thomas L. Fillmore[1]; Song Nie[1]; Carrie D. Nicora[1]; H. Steven Wiley[1]; Karin D. Rodland[1]; Tao Liu[1]; Richard D. Smith[1]; Wei-Jun Qian[1]; *[1]PNNL, Richland, WA*

MP 538 **An Objective Cross-Platform Comparison between MRM and PRM Based Quantitative Plasma Proteomic Workflows Reveals Similar Sensitivity and Reproducibility**; Vincent R. Richard[1]; Andre M. LeBlanc[1]; Christoph H. Borchers[1, 2, 3, 4]; *[1]JGH Proteomics Centre, Lady Davis Institute, McGill University, Montreal, QC, Canada; [2]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [3]Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; [4]Dept. of Oncology, Segal Cancer Centre, Jewish General Hospital, McGill University, Montreal, QC, Canada*

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MP 539 **Multi-omic Approach for Characterizing Plant Peptide Hormone Signaling Pathways That Regulate Cell Expansion**; Greg Sabat[1]; Gregory A. Barrett-Wilt[1]; Michael R. Sussman[1]; *[1]University of Wisconsin, Madison, WI*

MP 540 **Engineered Resistance to a Bean Fungal Disease against Proteins Found by Mass Spectrometry**; Bret Cooper; *USDA-ARS, Beltsville, MD*

MP 541 **Analysis of Canadian Wheat Varieties Low Molecular Weight Glutenin Subunits Relative to Gluten Strength : A Genotype x Environment Study**; Dave Hatcher[1]; Raymond Bacala[1]; *[1]Grain Research Lab, Canadian Grain Commission, Winnipeg, MB*

MP 542 **Investigation of Kinase-Substrate Networks in Photosynthetic Organisms**; Megan M. Ford[1]; Alex Chao[1]; Chris A. Broberg[1]; Leslie M. Hicks[1]; *[1]University of North Carolina, Chapel Hill, NC*

MP 543 **The Proteomic Profile of Rice Mitosis under Drought Stress**; Paul A. Haynes[1]; Yunqi Wu[1]; Mehdi Mirzaei[1]; Dana Pascovici[2]; Brian J. Atwell[3]; *[1]Dept of Chemistry and Biomolecular Sciences, Macquarie University, North Ryde, Sydney, Australia; [2]Australian Proteome Analysis Facility, Macquarie University, North Ryde, Sydney, Australia; [3]Dept of Biological Sciences, Macquarie University, North Ryde, Sydney, Australia*

MP 544 **Global Analysis of Native Protein Complexes inCyanothecesp. ATCC 51142 using Label-Free Quantitative Proteomic Profiling**; Uma Aryal[1]; Victoria Hedrick[1]; Tiago José Paschoal Paschoal Sobreira[1]; Christina R Ferreira[1]; Ding Ziyun[2]; Daisuke Kihara[2]; Louis Sherman[3]; *[1]Bindley Bioscience Center, Purdue University, West Lafayette, IN; [2]Department of Computer Science, Purdue University, West Lafayette, United Arab Emirates; [3]Department of Biological Sciences, Purdue University, West Lafayette, IN*

MP 545 **Leaf Spray Mass Spectrometry for Soybean Metabolomics**; Troy Wood[1]; Kevin Zemaitis[1]; Daniel Szczepankiewicz[1]; *[1]University at Buffalo, Buffalo, NY*

MP 546 **Ion Mobility and High Resolution Mass Spectrometry of Centella asiatica Extracts – Characterization and Quantification of Phytochemical Constituents**; Armando Alcazar Magana[1]; Maya Caruso[2]; Amala Soumyanath[2]; Joseph Quinn[2, 3]; Jan F. Stevens[4, 5]; Claudia S. Maier[1]; *[1]Department of Chemistry, Oregon State University, Corvallis, OR; [2]Department of Neurology, Oregon Health & Science University, Portland, OR; [3]Department of Neurology and Parkinson's Disease Research Education and Clinical Care Center, Portland, Or; [4]Department of Pharmaceutical Sciences, Oregon State University, Corvallis, OR; [5]Linus Pauling Institute, Oregon State University, Corvallis, OR*

MP 547 **Evaluation of ETD, HCD and CID Fragmentation for Phosphoproteomics of Grape (Vitis viniferaL.) Berries**; Liping Yang[1]; Satyanarayana Gouthu[2]; Laurent G. Deluc[2]; Claudia S. Maier[1, 3]; *[1]Department of Chemistry, Oregon State University, Corvallis, OR; [2]Department of Horticulture, Oregon State University,, Corvallis, OR; [3]Linus Pauling Institute, Oregon State University, Corvallis, OR*

MP 548 **Using Metabolomics to Uncover Metabolic Pathways Utilized in Nitrogen Stress and Plant-Microbe Interactions in Energy Sorghum**; Amy M. Sheflin[1]; Jessica E. Prenni[1]; Daniel P. Schachtman[2]; Rebecca Bart[3]; Thomas Brutnell[3]; Daniel Chitwood[3]; Asaph Cousins[4]; Jeffrey Dangl[5]; Ismail Dweikat[2]; Andrea Eveland[3]; Maria Harrison[6]; Stephen Kresovich[7]; Peng Liu[8]; Todd Mockler[3]; Susannah Tringe[9]; Arthur Zygielbaum[2]; *[1]Colorado State University's Proteomics and Metabolomics Facility, Fort Collins, CO; [2]University of Nebraska-Lincoln, Lincoln, NE; [3]Donald Danforth Plant Science Center, St. Louis, MO; [4]Washington State University, Pullman, WA; [5]UNC-Chapel Hill, Chapel Hill, NC; [6]Boyce Thompson Institute, Ithaca, NY; [7]Clemson University, Clemson, SC; [8]Iowa State University, Ames, IA; [9]Joint Genome Institute-DOE, Walnut Creek, CA*

MP 549 **Proteomic Identification of BIK1 Direct Substrates that Mediate the Arabidopsisinnate Immunity**; Peipei Zhu[1]; Chuan-Chih Hsu[1]; Pengchang Wang[1]; Yanyan Du[1]; Jian-Kang Zhu[1]; W. Andy Tao[1]; *[1]Purdue University, West Lafayette, IN*

MP 550 **Paterno-Buchi (PB) Reaction Coupled with Tandem Mass Spectrometry for the Analysis of Plant Lipids and Their Isomers**; Leelyn Chong[1]; Zheng Ouyang[2, 3]; Yu Xia[2, 3]; *[1]Purdue University, West Lafayette, IN; [2]Purdue University, West lafayette, Indiana; [3]Tsinghua University, Beijing, Beijing*

MP 551 **Investigation of Natural Products in Symbiotic Nitrogen-Fixing Root Nodules of Datisca glomerata by LC-MSn and Ion Tree Analysis using iTree**; Arpana Vaniya[1, 2]; Sajjan S. Mehta[2]; Kai Battenberg[3]; Alison Berry[3]; Oliver Fiehn[2]; *[1]UC Davis Department of Chemistry, Davis, CA; [2]West Coast Metabolomics Center, Davis, CA; [3]UC Davis Department of Plant Sciences, Davis, CA*

MP 552 **Advances in the Use of *in vivo* Crosslinking and Immunoaffinity Purification-Mass Spectrometry to Provide Insights into Unconventional Protein Secretion**; Tricia C. Ho[1]; Kevin Blackburn[1]; John D. Williamson[1]; Michael B. Goshe[1]; *[1]NC State University, Raleigh , NC*

MP 553 **Proteomic Analysis of H2S Induced Protein S-Sulfhydration in Arabidopsis thaliana**; Yixiang Zhang[1, 2]; Xuhong Yu[3]; Hui Peng[1, 4]; David P. Giedroc[1, 4]; Scott D. Michaels[3]; Jonathan Trinidad[1, 2]; *[1]Department of Chemistry, Indiana Univeristy, Bloomington, IN; [2]Laboratory for Biological Mass Spectrometry, Indiana University, Bloomington, IN; [3]Department of Biology, Indiana University, Bloomington, IN; [4]Department of Molecular and Cellular Biochemistry, Indiana University, Bloomington, IN*

MP 554 **GC-MS and UHPLC-HRMS Analysis of Aechmea Magdalenae Rhizome against E. coli and S. aureus**; Mirna Giron[1]; Quintin Ferraris[1]; Anima Ghosal[1]; Dil Ramanathan[2]; *[1]Kean University, Union, NJ; [2]Kean University, Union, NJ*

MP 555 **Detecting the "Un-natural" in Natural Products**; Jimmy Yuk[1]; Dhavalkumar Narendrabhai Patel[2]; Sukhdev Bangar[3]; Yun Wang Alelyunas[1]; Jayne Kirk[4]; Giorgis Isaac[1]; Mark Wrona[1]; *[1]Waters Corporation, Milford, MA; [2]Waters Pacific Private Ltd, Singapore, Singapore; [3]Waters Corporation, Beverly, MA; [4]Waters Corporation, Wilmslow, UK*

MP 556 **Chemical Fingerprinting of Essential Oils from Conifer Needles by ESI/APPI FT-ICR Mass Spectrometry**; Omolara Mofikoya[1]; Marko Mäkinen[1]; Janne Jänis[1]; *[1]Department of Chemistry, University of Eastern Finland, Joensuu, Finland*

MP 557 **Divergence in Phenolic Secondary Metabolites and Tyrosine Hyperaccumulation among Populations in the Inga umbellifera clade (Fabaceae), a Tropical Tree**; Gordon C. Younkin[1]; Dale L. Forrister[1]; Gabrielle Ghabash[1]; Phyllis D. Coley[1, 2]; Maria-Jose Endara[1]; James A. Nicholls[3]; R. Toby Pennington[4]; Kyle G. Dexter[3]; Graham N. Stone[3]; Catherine A. Kidner[4]; Thomas A. Kursar[2, 5]; *[1]University of Utah, Salt Lake City, UT; [2]Smithsonian Tropical Research Institute, Panama City, Panama; [3]University of Edinburgh, Edinburgh, UK; [4]Royal Botanic Garden Edinburgh, Edinburgh, UK; [5]University of Utah, Salt Lake City, UT*

MP 558 **Temporal Proteome and Metabolome Profiling of Water-Deficit Stress Responses in Populus Leaves**; Paul E. Abraham[1]; Daniel A. Jacobson[1]; Robert L. Hettich[1]; Gerald A. Tuskan[1]; Timothy J. Tschaplinski[1]; *[1]Oak Ridge National Laboratory, Oak Ridge , TN*

MP 559 **Identifying and Characterizing Plant-Derived Cyclic Peptides via High Resolution LC-MS/MS**; Nicole C Parsley[1]; Christine L Kirkpatrick[1]; Leslie M Hicks[1]; *[1]University of North Carolina at Chapel Hill, Department of Chemistry, Chapel Hill, NC*

MP 560 **Comparison of Different Offline Fractionation Techniques for Label Free Proteome Profiling of Arabidopsis Leaf Tissue**; Julia Mergner[1]; Lucia Guettler[1]; Bernhard Kuster[1]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany*

MP 561 **Proteome Analysis of Brachypodium distachyon Leaves under Drought Stress with Timewise Variation**; Ozge Tatli[1]; Bahar Sogutmaz Ozdemir[2]; Gizem Dinler Doganay[1]; *[1]Istanbul Technical University, Istanbul, Turkey; [2]Yeditepe University, Istanbul, Turkey*

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MP 562 **Evidence that the Polyglutamine Aggregation Inhibitor QBP1 Interacts with Monomeric Ataxin-3 at a Novel Site**; Patrick Knight[1]; Theodoros Karamonos[1]; Sheena E Radford[1]; Alison E Ashcroft[1]; *[1]University of Leeds, Leeds, Yorkshire*

MP 563 **Assessing Conformational Heterogeneities of Beta-2 Microglobulin Pre-Amyloid Oligomers using Ion Mobility Mass Spectrometry**; Tyler Marcinko[1]; Richard W Vachet[1]; *[1]University of Massachusetts-Amherst, Amherst, MA*

MP 564 **Time-Resolve Mass Spectrometry with A Micromixing Tee Applied to Kinetic Studies of Cd2+ Binding to Methallothionein-2A**; Shiyu Dong[1]; Nicole Wagner[1]; David H Russell[1]; *[1]Texas A&M University, College Station, TX*

MP 565 **Characterization of Biotherapeutics by Native SEC-MS: from Cysteine-linked Antibody Conjugates to Megadalton Protein Assembly**; Jia Dong[1]; Suprit Deol[1]; Feng Wang[1]; Bryant Chau[1]; Karla Henning[1]; David Passmore[1]; *[1]Bristol-Myers Squibb, Redwood City, CA*

MP 566 **Interaction Proteomics on Glycine Receptor Interactome Reveal Novel Interactors: Implication in Inhibitory Neurotransmission in Brain Stem and Spinal Cord**; Sophie J.F. van der Spek[1]; Frank Koopmans[1]; Miguel A. Gonzalez-Lozano[1]; Roel van der Schors[1]; Ka Wan Li[1]; August B. Smit[1]; *[1]CNCR, VU Amsterdam, Amsterdam, Noord Holland*

MP 567 **Investigating Additional Functions of BMV Capsid Protein by Mass Spectrometry**; Alexander D. Jacobs[1]; Haley S. Hoover[2]; C. Cheng Kao[2]; David E. Clemmer[2]; *[1]Indiana University, Bloomington, IN; [2]Indiana University, Bloomington , IN*

MP 568 **Determining Ligand Interactions of Parvovirus with Fragment Antibodies and Transferrin Receptors using Charge Detection Mass Spectrometry**; Carmen Dunbar[1]; Heather Callaway[2]; Colin Parrish[2]; Martin Jarrold[1]; *[1]Indiana University, Bloomington , IN; [2]Cornell University, Ithaca, NY*

MP 569 **Separation and Quantification of Amyloid Beta Oligomers and Monomers Using a 2D-LC-MS/MS System**; Farid Jahouh[1]; Herman Borghys[2]; Filip Cuyckens[1]; Rob J Vreeken[1, 3]; *[1]Discovery Sciences, Janssen Pharmaceutica, Beerse, Belgium; [2]Neurosciences Department, Janssen Pharmaceutica, Beerse, Belgium; [3]M4I Institute - Maastricht University, Maastricht, Netherlands*

MP 570 **Novel Protein-Protein Interactions with Specific Functional Domains of RNA Polymerase II**; Whitney Smith-Kinnaman[1]; Asha Boyd[1]; Nada Alakhras[1]; Gabriela Mazur[2]; Lynn Bedard[3]; Amber Mosley[1]; *[1]Indiana University School of Medicine, Indianapolis, IN; [2]Indiana University−Purdue University Indianapolis, Indianapolis, IN; [3]DePauw University, Greencastle, IN*

MP 571 **Using Native Top-Down nESI FTICR-MS to Characterize the Interaction of Tau Protein with Assembly Modulator CLR01**; Michael Nshanian[1]; Joseph A Loo[1]; Piriya Wongkongkathep[1]; Gal Bitan[1]; *[1]UCLA, Los Angeles, CA*

MP 572 **Anti-apoptotic Bag-1S is Involved in Ubiquitin-Dependent Proteasomal Degradation by Forming a Complex with AAA ATPase, p97/VCP**; Sevilay Acar[1]; Nisan Can[1]; Tugba Kizilboga[1]; Ozge Tatli[1]; Gizem Dinler Doganay[2]; *[1]Istanbul Technical University, Istanbul, Turkey; [2]Istanbul*

MP 573 **Analysis of Oxygen Sensitive Nitrogenase Complexes using Native Mass Spectrometry**; Monika Tokmina-Lukaszewska[1]; Natasha Pence[1]; Rhesa Ledbetter[2]; Zhiyong Yang[2]; John Peters[3]; Lance Seefeldt[2]; Brian Bothner[1]; *[1]Montana State University, Bozeman, MT; [2]Utah State University, Logan, UT; [3]Washington State University, Pullman, WA*

MP 574 **The Effect of Protein Concentration and Metal Content on Calprotectin Oligomerization as Revealed by Native Electrospray Ionization Mass Spectrometry**; Boone M Prentice[1]; Benjamin A Gilston[2]; Kevin L. Schey[2]; Walter J Chazin[2]; Richard M. Caprioli[2]; *[1]Vanderbilt University, Nashville, TN; [2]Vanderbilt University, Nashville, TN*

MP 575 **Identification of Interaction Partners of Protein Phosphatase 2A in Human Skeletal Muscle using Label Free Mass spectrometry**; divyasri damacharla[1]; Zhengping Yi[2]; Xiangmin Zhang[2]; Danjun ma[1]; Yue Qi[1]; berhane seyoum[1]; Abdullah mallisho[1]; sorin Dragichi[1]; Michael Caruso[1]; *[1]Wayne State University, Detroit, MI; [2]Wayne State University, Detroit, MI*

MP 576 **Limited Charge Reduction Coupled IM-MS Reveals Distinct Models of Biopolymers Interaction between Protamine and Heparin**; Yunlong Zhao[1]; Igor A. Kaltashov[2]; *[1]University of Massachusetts Amherst, Amherst, MA; [2]University of Massachusetts-Amherst, Amherst, MA*

MP 577 **Identification of the 'Readers' of Histone Modification by Combination of DNA-templated Peptide Probe and Mass Spectrometry Analysis**; Xue Bai[1]; Congcong Lu[2]; Shanshan Tian[1]; Guijin Zhai[1]; Kai Zhang[1, 2]; *[1]Tianjin Medical University, Tianjin, Tianjin; [2]Nankai University, Tianjin*

MP 578 **Comparative Interactome Analysis of Multidrug-Resistant and Sensitive Pathogenic Bacteria Strains of Acinetobacter baumannii** ; Xuefei Zhong[1]; Xia Wu[1]; Juan D. Chavez[1]; Devin K Schweppe[1]; Arti T Navare[1]; Jimmy K Eng[1]; James E Bruce[1]; *[1]University of Washington, Seattle, WA*

MP 579 **Screening and Characterization of Nanobody-ABC-transporter Complexes using High-Mass Matrix-Assisted Laser Desorption/Ionization-Mass Spectrometry**; Martin Köhler[1]; Camilo Perez[2]; Kaspar Locher[2]; Renato Zenobi[1]; *[1]ETH Zurich, Department of Chemistry and Applied Biosciences, Zurich, Switzerland; [2]ETH Zurich, Institute of Molecular Biology and Biophysics, Zurich, Switzerland*

MP 580 **Investigation of GTP-Dependent K-Ras Oligomerization Using Native Top-Down Ultraviolet Photodissociation Mass Spectrometry**; M. Rachel Mehaffey[1]; Michael B. Cammarata[1]; Christopher L. Schardon[2]; Walter Fast[3]; Jennifer S. Brodbelt[1]; *[1]Department of Chemistry, University of Texas at Austin, Austin, TX; [2]Graduate Program in Biochemistry, University of Texas at Austin, Austin, TX; [3]Division of Chemical Biology and Medicinal Chemistry, College of Pharmacy, University of Texas at Austin, Austin, TX*

MP 581 **Interaction of Transcription Factor TEAD and Its DNA Response Element from C-MYC Promoter Studied by Structural Mass Spectrometry**; Ruzena Liskova[1, 2]; Lukas Slavata[1, 2]; Daniel Kavan[1, 2]; Karel Valis[1, 2]; Petr Man[1, 2]; Petr Novak[1, 2]; *[1]BIOCEV, Institute of Microbiology of the CAS, v.v.i., Vestec, Czech Republic; [2]Faculty of Science, Charles University, Prague, Czech Republic*

MP 582 **Determination of the Heparin-Binding Sites of RPTP-LARs Via HRFP-FPOP and LC-MS/MS**; Charles Mobley[1]; Pradeep Prabhakar[2]; Chelsea Suppinger[1]; Kelley Moremen[2]; Joshua Sharp[1]; *[1]University of Mississippi, Oxford, MS; [2]University of Georgia, Athens, GA*

MP 583 **Quantifying the Effects of Membrane Composition on Protein-Glycolipid Interactions Using Nanodiscs and Proxy Ligand ESI-MS**; Ling Han[1]; Elena Kitova[1]; John Klassen[1]; *[1]University of Alberta, Edmonton, AB, Canada*

MP 584 **Native Mass Spectrometry to Identify Stoichiometries and Stability of Protein-Ligand Complexes**; Sabine Wittig[1]; Marius Rutkauskas[2]; Ralf Seidel[2]; Carla Schmidt[1]; *[1]IWE ZIK HALOmem Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany; [2]Institute of Experimental Physics I Universität Leipzig, Leipzig, Germany*

MP 585 **Elucidating Cellular Locales by Crosslinking Mass Spectrometry**; Richard A. Scheltema[1, 2]; Fan Liu[1, 2]; Oleg Klykov[1, 2]; Sibel Bayrak[1, 2]; Barbara Steigenberger[1, 2]; Domenico Fasci[1, 2]; Albert J. R. Heck[1, 2]; *[1]Utrecht University, Utrecht, Netherlands; [2]Netherlands Proteomics Center, Utrecht, Netherlands*

MP 586 **Dynamic Protein Interactions and Post-Translational Modifications in Monocytes**; Annika Frauenstein[1]; Matthias Mann[1]; Felix Meißner[1]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany*

MP 587 **MS Study of Zinc-Binding to Mutant Forms of Amyloid-Beta Provide an Insight on the Early Mechanisms of Familial Alzheimer's Disease**; Maria I. Indeykina[1, 2, 3]; Alexey S. Kononikhin[1, 2, 3]; Igor A. Popov[1, 2, 3]; Aleksandra A. Kulikova[4]; Sergey A. Kozin[4]; Eugene (Evgeny) Nikolaev[2, 3, 5]; *[1]Emanuel Institute of Biochemical Physics of Russian Academy of Sciences, Moscow, Russia; [2]Institute for Energy Problems of Chemical Physics of RAS, Moscow, Russia; [3]Moscow Institute of Physics and Technology (State University), Dolgoprudnyj, Russia; [4]Engelhardt Institute of Molecular Biology, Moscow, Russia; [5]Skolkovo institute of science and technology, Skolkovo, Russia*

MP 588 **Analysis of a Reconstituted, Non-Covalent Type III-A CRISPR-Cas Complex using Native Mass Spectrometry**; Tina Y. Liu[1, 2]; Anthony T Iavarone[3, 4]; Jennifer A. Doudna[1, 2, 3, 5, 6]; *[1]Department of Molecular and Cell Biology, University of California, Berkeley, CA; [2]Howard Hughes Medical Institute, University of California, Berkeley, CA; [3]California Institute for Quantitative Biosciences, University of California, Berkeley, CA; [4]Department of Chemistry, University of California, Berkeley, CA; [5]Innovative Genomics Initiative, University of California, Berkeley, CA; [6]MBIB Division, Lawrence Berkeley National Laboratory, Berkeley, CA*

MP 589 **Mapping the HLA Antibody Interaction with Blue Paint**; William Hildebrand[1]; Virginie Sjoelund[1]; *[1]OUHSC, Oklahoma City, OK*

MP 590 **Development of an MS Approach for Characterizing Intracellular Proteins Interacting with a G Protein-Coupled Receptor Captured using Laser-Induced Photo-Activation**; Chen Qian[1, 2]; Melinda Hauser[2]; Tyler King[2]; Jeffrey Becker[2]; Robert Hettich[1]; *[1]Oak Ridge National Laboratory, Oak Ridge , TN; [2]University of Tennessee, Knoxville, TN*

MP 591 **High Throughput, Label- and Immobilization-Free Screening of Human Milk Oligosaccharides against Lectins**; Amr El-Hawiet[1, 2]; Yajie Chen[1]; Km Shams-Ud-Doha[1]; Elena N. Kitova[1]; John S. Klassen[1]; *[1]Alberta Glycomics Centre and Department of Chemistry,*

University of Alberta, Edmonton, Alberta; [2]Department of Pharmacognosy, Faculty of Pharmacy, Alexandria University, Alexandria, Egypt

MP 592 **Native Mass Spectrometry Reveals Endogenous Stoichiometric Control Governing Protein Complexation in Metabolism: A Case Study of Glycolytic Enzyme Triosephosphate Isomerase**; Luis F. Schachner[1]; Benjamin Des Soye[2]; Nicole A Haverland[2]; Josiah Hutton[2]; Owen Skinner[2]; Michael Jewett[2]; Philip Compton[2]; Neil L Kelleher[2]; *[1]Northwestern University, Evanston, IL; [2]Northwestern University, Evanston, IL*

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MP 593 **Large-scale Characterization and Quantitation of Citrullinated Proteins Involved in Restenosis by HCD Product Ion Triggered EThcD Mass Spectrometry**; Yatao Shi[1]; Zhengwei Chen[2]; Qing Yu[3]; Bowen Wang[4]; Matthew Glover[5]; Xudong Shi[6]; Lian-wang Guo[4]; Craig K. Kent[4]; Lingjun Li[5, 7]; *[1], Madison, Wisconsin; [2]Chemistry Department, University of Wisconsin Madison, Madison, WI; [3]Pharmacy School, University of Wisconsin-Madison, Madison, WI; [4]Davis Heart and Lung Research Institute, The Ohio State University, Columbus, OH; [5]School of pharmacy, University of Wisconsin Madison, Madison, WI; [6]Department of Surgery,University of Wisconsin-Madison, Madison, WI; [7]Department of chemistry, University of Wisconsin Madison, Madison, WI*

MP 594 **MS-compatible Subcellular Fractionation Protocol based on Phase Transfer Surfactants**; Takeshi Masuda[1]; Naoyuki Sugiyama[2]; Sumio Ohtsuki[1]; Yasushi Ishihama[2]; *[1]Kumamoto University, Kumamoto, Japan; [2]Kyoto University, Kyoto, Japan*

MP 595 **A Proteomics Approach to Characterize Trace Host Cell Protein Impurities in Drug Substance and Guide Purification Process Development**; Yu Zhou[1]; Sushmita Mimi Roy[1]; *[1]BioMarin Pharmaceutical Inc., Novato, CA*

MP 596 **Proteomic Analysis Identifies Novel Regulators of the ade6-M26 Meiotic Recombination Hotspot**; Aaron Storey[1]; Stephanie Byrum[1]; Mari K. Davidson[1]; Alan J Tackett[1]; Sam Mackintosh[1]; Wayne P. Wahls[1]; *[1]University of Arkansas for Medical Sciences, Little Rock, AR*

MP 597 **Microfluidic Nanoliter Sample Preparation Enables Deep Proteome Analysis of 10 Cells**; Ying Zhu[1]; Paul D Piehowski[2]; Rui Zhao[2]; Yufeng Shen[2]; Ronald J Moore[2]; Weijun Qian[2]; Richard D. Smith[2]; Ryan Kelly[2]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Pacific Northwest National Laboratory, Richland, WA*

MP 598 **Epitope Identification and Affinity Quantification of ßAmyloid Specific Antibodies using Online SPR-Biosensor- ESIMS**; Loredana Mirela Lupu[1, 2]; Hendrik Rusche[3, 4]; Zdenek Kukacka[3]; Yannick Baschung[2, 3]; Marry Murphy[5]; Jeff Bornheim[5]; Michael Przybylski[3, 4]; *[1]Steinbeis Center for Biopolymer Analysis & Biomedical Mass Spectrometry, Ruesselsheim am Main, Germany; [2]Proteom Zentrum Röstock, Institut für Immunologie, Universitätmedizin Röstock, Rostock, Germany; [3]Steinbeis Centre Biopolymer Analysis and Biomedical Mass Spectrometry, Ruesselsheim am Main, Germany; [4]University of Konstanz, Department of Chemistry, Konstanz, Germany; [5]Reichert- Ametek Technologies, Buffalo, NY*

MP 599 **Database Independent Protein Sequencing (DiPS) Enables Full-Length *de-novo* Protein and Antibody Sequence Determination**; Alon Savidor[1]; Rotem Barzilay[1]; Dalia Elinger[1]; Yosef Yarden[2]; Moshit Lindzen[2]; Alexandra Gabashvili[1]; Ophir Adiv Tal[1]; Yishai Levin[1]; *[1]The Nancy and Stephen Grand Israel National Center for Personalized Medicine, Weizmann Institute of Science, Rehovot, Israel; [2]Department of Biological Regulation, Weizmann Institute of Science, Rehovot, Israel*

MP 600 **Optimization of a Promising Sample Preparation Protocol, Tube-Gel, for High Throughput Quantitative Proteomics**; Leslie Muller[1]; Luc Fornecker[1]; Alain Van Dorsselaer[1]; Sarah Cianferani[1]; Thierry Rabilloud[2]; Christine Carapito[1]; *[1]Laboratoire de Spectrométrie de Masse BioOrganique, University of Strasbourg, Strasbourg, France; [2]Laboratoire de Chimie et Biologie des Métaux, UMR 5249, iRTSV/LCBM, CEA, Grenoble, France*

MP 601 **'Boxcar' Method Enables Single Shot Proteomics at a Depth of 10,000 Proteins in 100 Minutes on a Hybrid Quadrupole-Orbitrap Instrument**; Florian Meier[1]; Philipp E Geyer[1, 2]; Juergen Cox[1]; Matthias Mann[1, 2]; *[1]Max-Planck Institute of Biochemistry, Martinsried, Germany; [2]NNF Center for Protein Research, Copenhagen, Denmark*

MP 602 **Ion 'Supercharging' for Improving Bottom-Up Protein Analysis by Liquid-Chromatography Mass Spectrometry**; Muhammad Zenaidee[1]; William A. Donald[2]; Mark J. Raftery[3]; Sydney Liu Lau[3]; *[1], Kensington, NSW; [2]University of New South Wales, Sydney, Australia; [3]Bioanalytical Mass Spectrometry, Sydney, NSW*

MP 603 **Scanning the Human Proteome for Multi-cistronic Genes**; Samuel Smukowski[1]; Xiaofei Du[2]; Daniel PH Pastor[2]; Jack D Godfrey[2]; Eshaan Rao[2]; Christopher M Gomez[2]; Jeffrey N Savas[3]; *[1]Northwestern University, Chicago, IL; [2]University of Chicago, Chicago, IL; [3]Northwestern University, Chicago, IL*

MP 604 **Isolated Pseudomonas aeruginosa from Mining Site: Proteome Changes Due to the Copper**; Cristiano José de Andrade[1, 2]; Meriellen Dias[1, 2]; Lidiane Maria de Andrade[1, 2]; Camila Delarmelina[3]; Marta Cristina Teixeira Duarte[3]; Maria Anita Mendes[1, 2]; Claudio Augusto Oller do Nascimento[1, 2]; *[1]Universidade de São Paulo - USP, Sao Paulo, South America; [2]Dempster Mass Lab- POLI- USP, Sao Paulo, Brazil; [3]Chemical, Biological and Agricultural Pluridisciplinary Research Center (CPQBA); University of Campinas – Brazil, Campinas, Brazil*

MP 605 **Diethylaminoethyl Sepharose (DEAE-Sepharose) Microcolumn for Glycopeptides Enrichment**; He Zhu[1]; Cheng Ma[2]; Peng George Wang[2]; *[1], Atlanta, GA; [2]Georgia State University, Atlanta, GA*

MP 606 **Analysis of Specific Synaptic Proteomes in Rodent Models ofAutism Spectrum Disorder**; Yi-Zhi Wang[1]; Samuel N Smukowski[1]; Kira A Cozzolino[1]; Jeffrey N Savas[1]; *[1]Northwestern University, Chicago, IL*

MP 607 **Proteome-wide Characterization of Metabolic Drugs AICAR and Metformin by Thermal Shift Assays**; Katherine A Overmyer[1]; Harald Marx[1]; Alex S Hebert[1]; Michael S Westphall[1]; Joshua J. Coon[1]; *[1]University of Wisconsin Madison, Madison, WI*

MP 608 **Comparison of Proteomic Profile of the Aspergillus niger Fungus (ATCC 11414 and Savage) Growing in Presence of Copper.**; Meriellen Dias[1, 2]; Lidiane Maria de Andrade[1, 2]; Enrique Eduardo Rozas Sanchez[1, 2]; Maria Anita Mendes[1, 2]; *[1]Universidade de São Paulo - USP, Sao Paulo, South America; [2]Dempster Mass Lab- POLI- USP, Sao Paulo, Brazil*

MP 609 **SAVControl: A Computational Framework for Quality Control of Variant Peptide Detection in Shotgun Proteomics**; Xinpei Yi[1]; Bo Wang[2]; Zhiwu An[1]; Fuzhou Gong[1]; Jing Li[2]; Yan Fu[1]; *[1]Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing, China; [2]Department of Bioinformatics and Biostatistics, School of Life Sciences and Biotechnology, Shanghai Jiao Tong University, Shanghai, China*

MP 610 **Automated Reproducible High-Throughput Proteome Analysis using Magnetic HILIC Microparticles**; Stoyan Stoychev[1]; Previn Naicker[1]; Isak Gerber[1]; Sipho Mamputha[1]; Justin Jordaan[2]; *[1]CSIR Biosciences, Pretoria, Gauteng; [2]ReSyn Biosciences, Pretoria, South Africa*

MP 611 **Trinity P1 Mixed Mode Chromatography Enables Streamlined MS Compatible Orthogonal Peptide Fractionation**; Peng Yu[1]; Mathias Wilhelm[1]; Daniel P Zolg[1]; Xuefei Sun[2]; Andreas Huhmer[3]; Bernhard Kuster[1, 4, 5]; *[1]Technical University of Munich, Freising, Germany; [2]Thermo Fisher Scientific, Sunnyvale, CA; [3]Thermo Fisher Scientific, San Jose, CA; [4]Center for Integrated Protein Science Munich, Freising, Germany; [5]Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany*

MP 612 **Project Julienne: Improved Quantitative Detection of Protein Isoforms, Post Translational Modifications and Total Proteome Coverage**; Thomas Clark[1]; Greg Stacey[1]; Nikolay Stoynov[1]; Leonard Foster[1]; *[1]UBC, Vancouver, BC, Canada*

MP 613 **High-throughput Orthogonal Validation of Plasma Membrane-Associated Networks by Differential Centrifugation**; Emmanuel E Ojefua[1]; Vincent C Chen[1]; *[1]Brandon University, Department of Chemistry, Brandon, MB*

MP 614 **The Loss-Less and Nano-Flow SPIDER Fractionator for High Sensitivity, High Coverage Proteomics**; Nils A. Kulak[1]; Philipp E Geyer[2]; Garwin Pichler[1]; Matthias Mann[2]; *[1]PreOmics, Planegg/Martinsried, Bavaria; [2]Max Planck Institute of Biochemistry, Martinsried, Germany*

MP 615 **Progress in Electrochemical Reduction of Disulfide Bonds in MS Proteomics**; Jean-Pierre Chervet [1]; Pablo Sanz de la Torre[1]; Hendrik-Jan Brouwer[1]; Nico Reinhoud[1]; Martin Eysberg[2]; *[1]Antec Scientific, Zoeterwoude, Netherlands; [2]Antec Scientific (USA), Boston, MA*

MP 616 **Highly Selective and Large Scale Mass Spectrometric Analysis of 4-Hydroxynonenal Modification via Fluorous Derivatization and Fluorous Solid-Phase Extraction**; Haojie Lu; *, Shanghai, Shanghai*

MP 617 **Creation and Improvement of Software Tools for Kinetic Proteomics Analysis**; Bradley Naylor[1]; Richard H Carson[2]; Marcus Hadfield[2]; John C Price[2]; *[1]Brigham Young University, Provo, UT; [2]Brigham Young University, Provo, UT*

MP 618 **Infrared Laser Desorption Capture Coupled with Ion Mobility-Mass Spectrometry and Chemometric Deconvolution for Analysis of Biological Tissues**; Michael E. Pettit[1]; Raul A. Villacob[1]; Matthew R. Brantley[1]; Fabrizio Donnarumma[2]; Kermit K. Murray[2]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX; [2]Louisiana State University, Baton Rouge, LA*

MP 619 **Affi-BAMS: A High Throughput Immunoaffinity Enrichment Assay with Detection by LAESI MS and MALDI MS**; Callee Walsh[1]; Erin H. Seeley[1]; Vladislav Bergo[2]; *[1]Protea Biosciences, Morgantown, WV; [2]Adeptrix Corp, Beverly, MA*

MP 620 **Evaluating the Performance of an Automated, Inexpensive Hood Robot by Developing an Open-Source, Python-Scripted In-Gel Digestion Workflow for Bottom-Up Proteomics**; Roasa Mehmood[1]; Ryan D. Leib[1]; Allis S. Chien[1]; Christopher M. Adams[1]; *[1]Stanford University Mass Spectrometry, Stanford, CA*

MP 621 **Reference Materials for Proteomic Investigations**; David M Bunk[1]; Ashley Beasley-Green[2]; Candice Johnson[2]; Lisa E. Kilpatrick[2]; Mark S. Lowenthal[2]; Karen W. Phinney[2]; *[1]NIST, Gaithersburg, MD; [2]National Institute of Standards and Technology, Gaithersburg, MD*

MP 622 **Proteome Signal Amplification Using TMT Multiplexing and a Carrier/Reference Strategy**; Paul M. Stemmer[1]; Nicholas J. Carruthers[2]; Joseph A. Caruso[1]; D. Randy Armant[1]; Sascha Drewlo[1]; *[1]Wayne State University, Detroit, MI; [2]Wayne State University, Detroit, MI*

MP 623 **A Synergistic Approach: Combining Label-Free Proteomics and MRM Techniques in a Single Method to Advance Health Care**; Bruce E. Wilcox[1]; Ryan W. Benz[1]; Phong Cun[1]; William F. Smith[1]; *[1]Applied Proteomics, San Diego, CA*

MP 624 **Investigating Protease Multiplexing to Improve Sequence Coverage in Bottom-Up Proteomics**; Jan Schrader[1]; Assa Yeroslaviz[1]; Anja Wehner[1]; Juergen Cox[1]; Nagarjuna Nagaraj[1]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany*

MP 625 **Identification of High pI-High Charge Peptides Using Capillary Electrophoresis Mass Spectrometry**; Tatiana N. Boronina [1]; Robert N. Cole[2]; Robert N. O'Meally[1]; *[1]Johns Hopkins School of Medicine, Baltimore , MD; [2]Johns Hopkins University School of Medicine, Baltimore, MD*

MP 626 **Mapping of T-Cell Surface N-Glycosylation**; Paul Kodama[1]; Mirna Mujacic[1]; Tom Kowski[1]; Ken Prentice[1]; *[1]Juno Therapeutics, Seattle, WA*

MP 627 **Capillary Electrophoresis – Mass Spectrometry Analysis of Histatin 5 and Its Analogs**; Yan Wang[1]; Svetlana P. Ikonomova[2]; Amy J. Karlsson[2]; Fahim C. Zarrin[3]; James Xia[3]; *[1]Proteomics Core Facility, University of Maryland, College Park, MD; [2]Department of Chemical and Biomolecular Engineering, University of Maryland, College Park, MD; [3]CMP Scientific, Corp., Brooklyn, NY*

MP 628 **An Automated Online Sample Preconcentration Platform for Bottom-Up Proteomics by Capillary Electrophoresis-Mass Spectrometry**; Zhenbin Zhang[1]; Elizabeth Peuchen[1]; Norman J Dovichi[1]; *[1]University of Notre Dame, Notre Dame, IN*

MP 629 **Open Sesame: Proteomics and Lipidomics of Oil and Fat Illuminants from Archaeological Lamps**; Anna Shevchenko[1]; Yimin Yang[2]; Andrea Schuhmann[1]; Bo Wang[3]; Changsui Wang[2]; Andrej Shevchenko[1]; *[1]MPI of Mol Cell Biology and Genetics, Dresden, Saxony; [2]University of Chinese Academy of Sciences, Beijing, China; [3]Xinjiang Uygur Autonomous Region Museum, Ürümchi, China*

MP 630 **Characterizing the Inhibitory Postsynaptic Proteome Directly from Mouse Brain Tissue using *in vivo* BioID Proximity Labeling and label Free Quantitation**; Erik J. Soderblom[1]; Akiyoshi Uezu[2]; M. Arthur Moseley[1]; Scott H. Soderling[2]; *[1]Proteomics and Metabolomics Shared Resource, Duke University School of Medicine, Durham , NC; [2]Department of Cell Biology, Duke University School of Medicine, Durham, NC*

MP 631 **Proteomic of microalgaeChlorella kessleri Cultivation under Stressed Condition Induced by Copper Ions**; Lidiane Maria Andrade[1, 2]; Meriellen Dias[1, 2]; Cristiano José Andrade[1, 2]; Maria Anita Mendes[1, 2]; Claudio Augusto Oller do Nascimento[1, 2]; *[1]Universidade de São Paulo - USP, Sao Paulo, South America; [2]Dempster Mass Lab- POLI- USP, Sao Paulo, Brazil*

MP 632 **Evaluation of a Modified Q Exactive HF for Shotgun Proteomics**; Christian Kelstrup[1]; Dorte B Bekker-Jensen[1]; Tabiwang Arrey[2]; Alexander Harder[2]; Jesper V. Olsen[1]; *[1]CPR, University of Copenhagen, Copenhagen, Denmark; [2]Thermo Fisher Scientific, Bremen, Germany*

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MP 633 **Utilizing an Accurate Mass and Retention Time Library to Facilitate Bio-Marker Discovery in the Human Cerebrospinal Fluid Proteome**; Cole Michel[1]; Richard Reisdorph[1]; Enrique Alvarez[1]; Vadiraja Bhat[2]; Paul Goodley[3]; Nichole Reisdorph[1]; *[1]University of Colorado Anschutz Medical Campus, Aurora, CO; [2]Agilent Technologies, Inc, Wilmington, DE; [3]Agilent Technologies, Inc., Wilmington, DE*

MP 634 **Relative Protein Quantification of a Contrived Mixture with Fusion MS2 and MS3-SPS TMT10-Plex Data**; Candace R. Guerrero[1]; Todd W. Markowski[2]; Alan J. Zimmerman[2]; Kristin L. M. Boylan[1]; Susan K. Van Riper[1]; Leeann Higgins [2]; Amy P. N. Skubitz[1]; Timothy Griffin[1]; *[1]University of Minnesota, Minneapolis, MN; [2]University of Minnesota, St. Paul, MN*

MP 635 **Protein Isoform Quantitation in Complex Proteomic Data**; Casimir Bamberger[1]; Salvador Martínez-Bartolomé[1]; Miranda Montgomery[1]; Sandra Pankow[1]; John D. Hulleman[2]; Jeffery W. Kelly[1]; Clara Moon[1]; Dennis Wolan[1]; John R. Yates III[1]; *[1]The Scripps Research Institute, La Jolla, CA; [2]University of Texas Southwestern Medical Center, Dallas, TX*

MP 636 **Post Immuno-Enrichment On-Bead Digestion for Protein Quantification using immuno-MALDI (iMALDI)**; Huiyan Li[1]; Robert Popp[1]; Bjorn Frohlich[1]; Christoph H. Borchers[1, 2]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

MP 637 **Absolute Quantification using Targeted Mass Spec Assays with Panorama and Skyline**; Nicholas Shulman[1]; Josh Eckels[2]; Vagisha Sharma[1]; Daniel S. Spellman[3]; Kristin Wildsmith[4]; Shadi Toghi Eshghi[4]; Jacob D Jaffe[5]; Michael J MacCoss[1]; Brendan MacLean[1]; *[1]University of Washington, Department of Chemistry, Seattle, WA; [2]LabKey, San Diego, CA; [3]Merck & Co., West Point, PA; [4]Genentech, Inc, South San Francisco, CA; [5]Broad Institute, Cambridge, MA*

MP 638 **SPEAQ: A Software Tool for Absolute Protein Quantitation Based on Peptide Quantitative Efficiency Learning**; Qiang Zhi Gao[1]; Cheng Chang[2]; Yan Fu[1]; Hong Xiao Qian[2]; Ping Yun Zhu[2]; *[1]National Center for Mathematics and Interdisciplinary Sciences, Key Laboratory of Random Complex Structures and Data Science, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing, China; [2]State key Laboratory of Proteomics, National Center for Protein Sciences Beijing, Beijing Proteome Research Center, National Engineering Research Center for Protein Drugs, Beijing, China*

MP 639 **Elaboration towards the Regulatory Mechanism of Phase Shift in Clostridium acetobutylicum with a Combinational Strategy of Omics**; Nannan Kong[1, 2]; Jingjing Zhao[3]; Qingfei Pan[1, 2]; Xiaomin Lou[1]; Jin Zi[2]; Lin Wu[1]; Yan Ren[2]; Quanhui Wang[1]; Siqi Liu[2]; *[1]Beijing Institute of Genomics, Chinese Academy of Sciences, Beijing, China; [2]BGI-Shenzhen, Shenzhen, China; [3]Diabetes and Obesity Center, U of L, Louisville, KY*

MP 640 **A Silk Road to Modern Translational Proteomics – SOPs based Comprehensive Proteome Profiling and Reproducible Quantitation**; Yue Xuan[1]; David Sarracino[2]; Sebastien Gallien[3]; Scott Peterman[2]; Pedro Navarro[1]; Heather Sumner[4]; *[1]Thermo Fisher Scientific, Bremen, Germany; [2]Thermo Fisher Scientific BRIMS Center, Cambridge, MA; [3]Thermo Fisher Scientific, Courtaboeuf, France; [4]Thermo Fisher Scientific, San Jose, CA*

MP 641 **Dual and Triple Reporter Ion Combinatorial Isobaric Reagents: 16-Plex and Beyond**; Craig Braun[1, 2]; Brian K Erickson[2, 3]; Gregory H Bird[4]; Steve P Gygi[3]; *[1]Havard Medical School, Boston, MA; [2]IQ Proteomics, LLC, Brookline, MA; [3]Harvard Medical School, Boston, MA; [4]Dana Farber Cancer Institute, Boston, MA*

MP 642 **Isobaric Tag-Based Multi-Dimensional Quality Assessment Standards for SPS-MS3 Analyses: Maximizing Quantifications, while Minimizing Interference**; Joao A Paulo[1]; Steven P. Gygi[1]; *[1]Harvard Medical School, Boston, MA*

MP 643 **Multiplex Quantitative Analysis using NeuCode SILAC Metabolic Labeling of Signaling Protein Targets**; Ryan Bomgarden[1]; Kratika Singhal[1]; Bhavin Patel[1]; Rosa Viner[2]; Seema Sharma[3]; Juergen Cox[4]; Joshua Coon[5]; JOHN C. ROGERS[1]; *[1]Thermo Fisher Scientific, Rockford, IL; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, San Jose, CA; [4]Max Planck Institute of Biochemistry, Martinsried, Germany; [5]University of Wisconsin, Madison, WI*

MP 644 **Combined Proteomic and RNA Expression Analysis of Laser Ablation Extracted Tissue**; Chao Dong[1]; Kelin Wang[1]; Fabrizio Donnarumma[1]; Scott W. Herke[1]; Michael E. Pettit[2]; Touradj Solouki[2]; Kermit K. Murray[1]; *[1]Louisiana State University, Baton Rouge, LA; [2]Baylor University, Waco, TX*

MP 645 **Optimization of Multi-notch MS3 Technique for Accurate Quantification with Dimethyl Amino Acid-based Isobaric Tags**; Yusi Cui[1]; Qing Yu[2]; Lingjun Li[1, 2]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI*

MP 646 **A Rapid Digestion Protocol for the Preparation of Complex Proteomic Samples**; Kevin Cook[1]; Sergei Saveliev[1]; Marjeta Urh[1]; Michael M Rosenblatt[1]; *[1]Promega Corporation, Madison, WI*

MP 647 **Active Enzyme Characterization using a Two-Dimensional IsobaricLabeling Activity-Correlated Quantitative Proteomics Platform(2D-TMT-ACPP)**; Hongyan Ma[1]; Toni Woodard[2]; Si Wu[2]; *[1]Oklahoma University, Norman, OK; [2]University of Oklahoma, Norman, OK*

MP 648 **IonStar-Mine: Reproducible, Fractionation-Free Measurement of 8000+ Unique Proteins in 100 Biological Samples with High Accuracy, Precision and <1% Missing Data**; Shichen Shen[1]; Jun Li[1]; Xiaomeng Shen[2]; Chengjian Tu[1]; Jun Qu[1]; *[1]University at Buffalo, Buffalo, NY; [2]Amgen, South San Francisco, CA*

MP 649 **Measuring Mitochondrial Protein Expression by Repeated Reinterrogation of LC-High Resolution Full Scan MS Datasets**; Caroline Kinter[1]; Zachary Young[1]; Luke Szweda[1]; Michael Kinter[1]; *[1]Oklahoma Medical Research, Oklahoma City, OK*

MP 650 **MIKE: A Peptide-Terminal Labeling Strategy for Precision Quantitative (meta)Proteomics**; Jacob Waldbauer[1]; Lichun Zhang[1]; Adriana Rizzo[1]; *[1]University of Chicago, Chicago, IL*

MP 651 **Novel Tagging Strategies for a Modified cPILOT Workflow with Higher Sample Multiplexing Capabilities**; Bushra Amin[1]; Renã A.S. Robinson[1]; *[1]University of Pittsburgh, Pittsburgh, PA*

MP 652 **Method for Measuring Protein Digestion Efficiency**; Carmen Fernandez-Metzler[1]; Bonnie Baker[1]; Richard King[1]; *[1]PharmaCadence Analytical Services, LLC, Hatfield, PA*

PROTEOMICS: TOP DOWN ANALYSIS I
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MP 653 **Online nano-2DLC Meets Top-Down MS: WCX/a×m/RPLC UVPD-HRMS Analysis of Histone Proteoforms**; Andrea Gargano[1]; Jared B Shaw[2]; Mowei Zhou[2]; Nikola Tolic[2]; Thomas Fillmore[2]; Ronald J Moore[2]; Ljiljana Pasa-Tolic[2]; *[1]Center for Analytical Chemistry Amsterdam, Amsterdam, Netherlands; [2]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Earth and Biological Sciences Directorate, Richland, WA*

MP 654 **Characterization of Histone Proteoforms Using Linear and Nonlinear Ion Mobility Separations with Electron Transfer Dissociation**; Pavel Shliaha[1]; Matthew Baird[2]; Mogens Nielsen[1]; Vladimir Gorshkov[1]; Andrew P. Bowman[2]; Julia L. Kaszycki[2]; Gordon A Anderson[3]; Todd D. Williams[4]; Ole N. Jensen[1]; Alexandre A. Shvartsburg[2]; *[1]University of Southern Denmark, Odense, Denmark; [2]Wichita State University, Wichita, KS; [3]GAA Custom Engineering, LLC, Benton City, WA; [4]University of Kansas, Lawrence, KS*

MP 655 **Automatic Selection of Discriminative Top-Down Mass Spectra with Diagno-Top: Application to the Differentiation of Bacterial Pathogens**; Diogo Borges Lima[1]; Mathieu Dupré[1]; André R F Silva[2]; Paulo Costa Carvalho[2]; Julia Chamot-Rooke[1]; *[1]Structural Mass Spectrometry and Proteomics Unit CNRS USR2000 Mass Spectrometry for Biology, Paris, France; [2]Computational Mass Spectrometry & Proteomics Group, Carlos Chagas Institute, Curitiba, Paraná, Brazil, Curitiba, Brazil*

MP 656 **"Active" Fungal Classification Utilizing Top-Down Proteomics**; Toni Woodard[1]; Zhe Wang[1]; Hongyan Ma[1];

Monica Stevenson[1]; Si Wu[1]; [1]*University of Oklahoma, Norman, OK*

MP 657 **Top-down Proteomics of Sarcomeres in Muscle-related Diseases**; Wenxuan CAI[1]; Zachery R Gregorich[1]; Ziqing Lin[1]; Zachary L Hite[1]; Takushi Kohmoto[1]; Ying Ge[1]; [1]*University of Wisconsin-Madison, Madison, WI*

MP 658 **High-Throughput Screening of Proteoform-Specific Binding of a Chemical Library Using a 24-plex Emitter Array Chip**; Geuncheol Gil[1]; Pan Mao[1]; Daojing Wang[1]; [1]*Newomics Inc., Emeryville, CA*

MP 659 **Increasing Dynamic Range and Sample Insight for Top-Down Proteoform Profling Analysis Using Data-Dependent MS/MS Experiments**; Pierre-Olivier Schmit[1]; Hans J.C.T. Wessels[2]; Marshall W. Bern[3]; Stephanie Kaspar-Schoenefeld[4]; Gary Kruppa[5]; [1]*Bruker France, Wissembourg, France;* [2]*Radboud Proteomics Center, Radboud University, Nijmegen, Netherlands;* [3]*Protein Metrics Inc., San Carlos, CA;* [4]*Bruker Daltonik GmbH, Bremen, Germany;* [5]*Bruker Daltonics, Billerica, MA*

MP 660 **A Multi-Modal Proteomics Strategy for Characterizing *in vitro* and *in vivo* p53 Modforms**; Caroline J DeHart[1]; Luca Fornelli[1]; Deepesh Agarwal[2]; Jacek W Sikora[1]; Dan Lu[2]; Philip D Compton[1]; Paul M Thomas[1]; Galit Lahav[2]; Jeremy Gunawardena[2]; Neil L Kelleher[1]; [1]*Proteomics Center of Excellence, Northwestern University, Evanston, IL;* [2]*Harvard Medical School, Boston, MA*

MP 661 **Top-down Online Electrospray Nano-Liquid Chromatography Orbitrap tandem Mass Spectrometry for Large Protein Identification in Cell Lysates**; Atim Atte Enyenihi[1]; Jason Neil[2]; Mark Fisher[1, 3]; [1]*ARUP Laboratories, Salt Lake City, UT;* [2]*Thermo Fisher Scientific, Cambridge, Massachusetts;* [3]*University of Utah, Salt Lake City, UT*

MP 662 **Simultaneous Label-free Quantitation of Proteoforms, Proteoform Ratios, and Total Protein up to 80kDa Split across Physiochemical Multidimensional Space**; John R Corbett[1, 2]; Daniel A Plymire[1]; Casey E Wing[1]; William S Phipps[1]; Steven M Patrie[1, 2]; [1]*UT Southwestern, Dallas, TX;* [2]*UT Dallas, Richardson, TX*

MP 663 **Higher Resolution in Top-Down Proteomics of Histones using Submicrometer Particles and Slip Flow**; Yiyang Zhou[1]; Ximo Zhang[1]; Luca Fornelli[2]; Philip Compton[2]; Neil L Kelleher[2]; Mary Wirth[1]; [1]*Purdue University-Department of Chemistry, West Lafayette, IN;* [2]*Northwestern University, Evanston, IL*

MP 664 **Intelligent Data Acquisition Strategies to Generate a Comprehensive Map of Intact Proteoforms in Budding Yeast using Deep Top-Down Sequencing**; Luca Fornelli[1]; Kristina Srzentic[1]; Timothy K. Toby[1]; Bryan P. Early[1]; Peter F. Doubleday[1]; Ryan T. Fellers[1]; Philip D. Compton[1]; Neil L. Kelleher[1]; [1]*Northwestern University, Evanston, IL*

MP 665 **Elucidation of Experimental Fragmentation Parameters Required for High-Throughput Proteoform Interrogation of Myelin Basic Protein**; William S Phipps[1]; John R Corbett[1]; Casey E Wing[1]; Lacey Purdue[1]; Daniel A Plymire[1]; Steven M Patrie[1]; [1]*University of Texas Southwestern Medical Center, Dallas, TX*

SMALL MOLECULES: QUANTITATIVE ANALYSIS I
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MP 666 **Chemical Analysis of ENDS vapor by LC/MS/MS-based Methodology**; Berk Oktem[1]; Charles A. Moran[1]; Samanthi I Wickramasekara[1]; [1]*US FDA, Silver Spring, MD*

MP 667 **Evaluation of THERMAL HISTORY of THERMOPLASTIC RESINS by THERMAL DESORPTION and PYROLYSIS COMBINED with DART-MS (TDP/DART-MS)**; Chikako Takei[1]; Kenichi Yoshizawa[1]; [1]*BioChromato, Inc., Fujisawa, Japan*

MP 668 **A Novel Approach to Minimize the Matrix Effect in the LC-MS/MS Method for Quantitation ofN-(2-Hydroxyethyl) succinimide in HumanUrine**; Dawei Zhou[1]; Shaoting Zhang[1]; Mohamed Osman[1]; Xinping Fang[1]; [1]*WuXi AppTec, Plainsboro, NJ*

MP 669 **HPLC Tandem Mass Spectrometric Quantitation of DNA-binding Polyamides in Cell Lysate**; Shanshan Guan[1]; Maria José Scuderi[1]; Benjamin J. Bythell[1]; James K. Bashkin[1]; [1]*University of Missouri-St. Louis, St. Louis, MO*

MP 670 **Selective Derivatization of Penicillamine Using DTNB: Improved Matrix Stability and LC-MS/MS Sensitivity**; Laurence Mayrand Provencher[1]; Vinicio Vasquez[1]; Milton Furtado[1]; Anahita Keyhani[1]; [1]*Altasciences, Laval, QC, Canada*

MP 671 **Screening and Quantification of Unapproved Dietary Supplements using Liquid Chromatography with Quadrupole-Orbitrap Mass Spectrometry**; Flavia Morales-Garcia[1]; Douglas M. Monroe[1]; Judith Hillegas[1]; Tracy A. Majkol[1]; Joan M. Nandrea[1]; Fenhong Song[2]; Aref El-Demerdash[1]; [1]*FDA, Lenexa, KS;* [2]*FDA, Rockville, MD*

MP 672 **Quantitative Analysis of Antiarrhythmic Drugsin Human PlasmaUsing a High Performance Triple Quadrupole Mass Spectrometer**; Keeley Murphy [1]; Claudia Martins[2]; Jonathan Josephs[2]; [1]*Thermo Fisher Scientific, San Jose , CA;* [2]*ThermoFisher, San Jose, CA*

MP 673 **Simultaneous Analysis of Emtricitabine, Tenofovir, and Efavirenz in Mouse Plasma, Amniotic Fluid, and Fetus Homogenate by UPLC-MS/MS**; Brenda L. Fletcher[1]; Melanie A. Rehder Silinski[1]; Reshan A. Fernando[1]; Veronica G. Robinson[2]; Suramya Waidyanatha[2]; [1]*RTI International, Research Triangle Park , NC;* [2]*Division of National Toxicology Program, NIEHS, Research Triangle Park, NC*

MP 674 **Tenofovir and Emtricitabine Quantification in Cervicovaginal Fluid: Collection Device Considerations in Support of Clinical Trials**; Teresa L. Parsons[1]; Lauren A. Seserko[1]; Mark A. Marzinke[1]; [1]*Johns Hopkins University School of Medicine, Baltimore, MD*

MP 675 **Resin-Coated Proppant Analysis for Formaldehyde Content by GC-MS Headspace, GC-VUV, and HPLC**; Jamie Schenk[1]; Doug D. Carlton Jr.[1, 2]; Jonathan Smuts[3]; Ty Hanna[4]; Danny Durham[4]; Kevin A. Schug[1]; [1]*University of Texas at Arlington, Arlington, TX;* [2]*CLEAR, Arlington, TX;* [3]*VUV Analytics, Inc., Austin, TX;* [4]*Apache Corporation, Houston, TX*

MP 676 **Method Conversion Tool between Instruments for Huge-Multiple MRM Transitions in LC-MS/MS Adopting the Conversion Factor of Collision Energy Voltage**; Akane Yamamoto[1]; Kazutaka Ikeda[2]; Yoshiki Tainaka[1]; Jun Watanabe[1]; [1]*Shimadzu Corporation, Kyoto, Japan;* [2]*RIKEN Center for Integrative Medical Sciences, Yokohama, Japan*

MP 677 **Highly Sensitive Simultaneous Quantitative Analysis of Estrone and Equilin from Plasma using LC/MS/MS**; Ashutosh Shelar[1]; Shailendra Rane[1]; Shailesh Damale[1]; Rashi Kochhar[1]; Purushottam Sutar[1]; Deepti Bhandarkar[1]; Anant Lohar[1]; Ajit Datar[1]; Pratap Rasam[1]; Jitendra Kelkar[1]; [1]*Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

MP 678 **Analysis of Glucosamine in Functioal Foods by LC-MS/MS**; Shin Yong Woon; *Ministry of Food & drug Safety, Cheongju, Chungcheongbuk-do*

MP 679 **LC/MS/MS Analysis of Fentanyl and Related Analogs Using Biocompatible Solid Phase Microextraction**; Candace Price[1]; Craig Aurand[1]; Sara Smith[1]; Emily Barrey[1]; [1]*MilliporeSigma, Bellefonte, PA*

MP 680 **Validation of a LC-MS/MS Method for Quantification of Digoxin in Triton X-100 Fortified Human Urine**; Damon Papac[1]; Brian M Murray[1]; James Vannicola[1]; Eugene F Miller[1]; Debra J Beck[1]; Kristine Wagner-Caruso[1]; [1]*Icon Plc, Whitesboro, NY*

MP 681 **Bionalysis of Fluticasone Propionate in Rabbit Plasma and Nasal/Sinus Tissue using Sensitive LC/MS/MS Methods**; Patrick Lin[1]; Bih-Hsiung Hsu[1]; [1]*PHARMout Lab, Sunnyvale, CA*

MP 682 **Simultaneous Determination of Dihydrotestosterone and Its Metabolites in Mouse Sera by LC-MS/MS with Chemical Derivatization**; Shashank Gorityala[1]; Shuming Yang[2]; Monica M Montano[3]; Yan Xu[1, 2]; *[1]Department of Chemistry, Cleveland State University, Cleveland, OH; [2]Case Comprehensive Cancer Center, Case Western Reserve University, Cleveland, OH; [3]Department of Pharmacology, Case Western Reserve University, Cleveland, OH*

MP 683 **Methods for the Determination of Drugs of Abuse in Oral Fluids Using an Automated Sample Preparation and uHPLC-MS/MS**; Larry M Mallis[1]; Brenna Espelien[1]; Erich Valenzuela[1]; Benjamin Moeller[1]; Yongquan Lai[1]; Jacob Jantzi[1]; Ryan Sheeler[1]; Philip Kuehl[1]; Jacob McDonald[1]; *[1]Lovelace Biomedical, Albuquerque, NM*

MP 684 **Capture Efficiency and Separation Performance of Dynamic pH Junction Focusing with Two On-Column Electrolyte Configurations in Capillary Electrophoresis Mass Spectrometry**; Lingyu Wang[1]; David D. Y. Chen[1]; *[1]University of British Columbia, Vancouver, BC, Canada*

MP 685 **A High Throughput UPLC-MS/MS Method for the Simultaneous Determination of Pravastatin and Rosuvastatin in Human Urine**; Feng-Ming James Chang[1]; Yuan-Shek Chen[1]; T. Ben Hsu[1]; *[1]QPS, LLC, Newark, DE*

MP 686 **Development of Combined LC-MS/MS Analysis for Citric Acid Cycle Intermediates, Acylcarnitines and Amino Acids**; Rohan R Shah[1]; Alisha House[1]; Erica M Fatica[1]; Yana Sandlers[1]; *[1]Cleveland State University, Department of Chemistry, Cleveland, OH*

MP 687 **Quantitation of 25OH Vitamin D2/D3 in Serum by a New SLE Method Coupled with LC-MS/MS**; Guotao Lu[1]; Warren Chen[1]; Wan Wang[2]; Suzi Qin[2]; Lei Yin[2]; *[1]Bonna-Agela Technologies, Wilmington, DE; [2]Bonna-agela Technologies Inc., Tianjin, China*

MP 688 **Analysis of GSK525762 and Its Major Oxidative Metabolites in Human Plasma using Liquid Chromatography with Tandem Mass Spectrometric Detection**; Zhilong Gong[1]; Chineta Barksdale[2]; Kelly Connelly[3]; Omobola Oladipupo[2]; Eric Thomas[2]; *[1]Covance Bioanalytical Svc, Indianapolis, IN; [2]Covance, Indianapolis, IN; [3]GlaxoSmithKline, Ware, UK*

MP 689 **A Special Preparation to Improve Phosphocholine Determination in Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS)**; jing Tan[1]; Chunyan Zhang[1]; Jason Gek Leong Neo[1]; Tania Setiawati[1]; *[1]Abbott Nutrition, Singapore*

SYSTEMS BIOLOGY I
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MP 690 **Web-Based Implementation of Kinase-Substrate Enrichment Analysis (KSEA) for Phosphoproteomics-Derived Kinase Activity Inference**; Danica Wiredja[1, 2]; Mehmet Koyutürk[1, 3]; Mark R. Chance[1, 2]; *[1]Center for Proteomics and Bioinformatics, Case Western Reserve University, Cleveland, OH; [2]Department of Nutrition, Case Western Reserve University, Cleveland, OH; [3]Department of Electrical Engineering and Computer Science, Case Western Reserve University, Cleveland, OH*

MP 691 **Protein Expressional Changes of Pseudomonas aeruginosa in Lactate-Supplemented Media**; Yeni P. Yung[1]; S Lee McGill[2]; Stephanie M. Cologna[1]; Hui Chen[1]; Ross P. Carlson[2]; Luke Hanley[1]; *[1]University of Illinois at Chicago, Chicago, IL; [2]Montana State University, Bozeman, MT*

MP 692 **Quantitative Proteomics of the Host-Pathogen Interplay duringSalmonellaTyphimurium Infection**; Jennifer Geddes-McAlister[1]; Felix Meissner[1]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany*

MP 693 **Proteogenomic Landscape of Squamous Cell Lung Cancer**; Paul A Stewart[1]; Robbert JC Slebos[1]; Eric A Welsh[1]; Ling Cen[1]; Yonghong Zhang[1]; Zhihua Chen[1]; Chia-Ho Cheng[1]; Fredrik Pettersson[1]; Anders Berglund[1]; Guolin Zhang[1]; Bin Fang[1]; Victoria Izumi[1]; Sean Yoder[1]; Katherine Fellows[1]; Yian Ann Chen[1]; Jamie K Teer[1]; Steven A Eschrich[1]; John M Koomen[1]; Eric B Haura[1]; *[1]Moffitt Cancer Center, Tampa, FL*

MP 694 **Pharmacoproteomic Characterisation of Human Colon and rectal Cancer**; Martin Frejno[1, 2]; Riccardo Zenezini Chiozzi[1, 3]; Mathias Wilhelm[1]; Heiner Koch[1, 4, 5, 6]; Runsheng Zheng[1]; Susan Klaeger[1, 5, 6]; Benjamin Ruprecht[1, 7]; Chen Meng[1]; Karl Kramer[1]; Anna Jarzab[1]; Stephanie Heinzlmeir[1, 5, 6]; Elaine Johnstone[2]; Enric Domingo[2, 8]; David Kerr[9]; Moritz Jesinghaus[10]; Julia Slotta-Huspenina[10]; Wilko Weichert[10]; Stefan Knapp[11]; Stephan M Feller[12, 13]; Bernhard Kuster[1, 5, 7, 14]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; [2]Department of Oncology, University of Oxford, Oxford, UK; [3]University of Rome, La Sapienza, Rome, Italy; [4]Max Planck Institute of Biochemistry, Martinsried, Germany; [5]German Cancer Consortium (DKTK), Munich, Germany; [6]German Cancer Research Center (DKFZ), Heidelberg, Germany; [7]Center for Integrated Protein Science Munich, Freising, Germany; [8]Wellcome Trust Centre for Human Genetics, University of Oxford, Oxford, UK; [9]Nuffield Division of Clinical Laboratory Sciences, University of Oxford, Oxford, UK; [10]Institute of Pathology, Technical University of Munich, Munich, Germany; [11]Institute of Pharmaceutical Chemistry, Goethe University, Frankfurt am Main, Germany; [12]Weatherall Institute of Molecular Medicine, University of Oxford, Oxford, UK; [13]Institute of Molecular Medicine, Martin-Luther-University, Halle (Saale), Germany; [14]Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany*

MP 695 **Integration of Metabolomics Data with Kinetic Models for Dynamic Flux Analysis and the Inference of Biochemical Mechanisms**; Zhen Qi; *, Lexington, KY*

MP 696 **12-week Aerobic, Resistance, and Combined Training Shows Posttranslational Regulation of Skeletal Muscle in Younger and Older Adults**; Matthew M. Robinson[1]; Surendra Dasari[2]; Adam R. Konopka[3]; Matthew L. Johnson[4]; S. Manjunatha[2]; Raul R. Esponada[5]; Rickey E. Carter[2]; Ian R. Lanza[2]; K. Sreekumaran Nair[2]; *[1]Oregon State University, Corvallis, OR; [2]Mayo Clinic, Rochester, MN; [3]Colorado State University, Fort Collins, CO; [4]Dexcom, San Diego, CA; [5]Sanford Health, Fargo, ND*

MP 697 **Longitudinal Metaproteomics Analysis of Premature Infant Intestinal Microbiota Reveals Early-Life Microbial and Host Metabolic Functions**; Weili Xiong[1]; Chris T Brown[2]; Matthew B Rogers[3]; Michael J Morowitz[3]; Jillian F Banfield[2]; Robert L Hettich[1]; *[1]Oak Ridge National Laboratory, Oak Ridge , TN; [2]Department of Earth and Planetary Science, UC, Berkeley, CA; [3]School of Medicine, University of Pittsburgh, Pittsburgh, PA*

MP 698 **Infrared Laser Ablation Sample Transfer with Conserved Biological Function**; Kelin Wang[1]; Matthew D. Baldone[1]; Fabrizio Donnarumma[1]; Kermit K. Murray[1]; *[1]Louisiana State University, Baton Rouge, LA*

MP 699 **Inferring Metabolic Function across Wildly Variable Gut Metaproteomes Derived from Crohn's Disease Patients Post Resection Surgery**; J. Alfredo Blakeley-Ruiz[1]; Alison R Erickson[2]; Weili Xiong[3]; Claire M. Fraser[4]; Robert L Hettich[3]; *[1]University of Tennessee, Knoxville, TN; [2]Harvard Medical School, Boston, MA; [3]Oak Ridge National Laboratory, Oak Ridge , TN; [4]University of Maryland School of Medicine, Baltimore, MD*

MP 700 **ProHits-viz: A Suite of Web-Tools for Visualizing Interaction Proteomics Data**; James D R Knight[1]; Hyungwon Choi[2]; Brian Raught[3]; Alexey I Nesvizhskii[4]; Anne-Claude Gingras[1, 5]; *[1]Lunenfeld-Tanenbaum Research Institute, Toronto, Ontario; [2]National University of Singapore, Singapore, Singapore; [3]Princess Margaret Cancer Centre, Toronto, ON, Canada; [4]Department of Pathology, University*

of Michigan, Ann Arbor, MI; [5]Department of Molecular Genetics, University of Toronto, Toronto, ON, Canada

MP 701 **Diagnosis of Ecosystem Adaptive Responses by Analysis of Hundreds of Peptide Biomarkers in the North Atlantic Ocean using Targeted Metaproteomics**; Mak Saito[1]; Matthew McIlvin[1]; Dawn Moran[1]; Luis Valentin[1]; Romain Huguet[2]; Shannon Eliuk[2]; Graeme McAlister[2]; Rod Johnson[3]; *[1]Woods Hole Oceanographic Inst., Woods Hole, MA; [2]ThermoFisher, San Jose, CA; [3]Bermuda Institute of Ocean Sciences, St. George's, Bermuda*

MP 702 **An Integrated Omics Approach to Characterize Complex Microbial Phenotype Behavior: Characterizing Bacterial Swarming**; Robert Hettich[1]; Richard J Giannone[1]; James Elkins[1]; Jenny Morrell-Falvey[1]; Abigail Tester[2]; Shawn R Campagna[2]; *[1]Oak Ridge National Laboratory, Oak Ridge , TN; [2]University of Tennessee, Knoxville, TN*

MP 703 **Leveraging Transcriptomic and Phosphoproteomic Data of Perturbed MCF10A Cells to Identify Downstream PTEN Events of Breast Cancer**; Chenwei Lin [1]; Richard Ivey[1]; Jacob J Kennedy[1]; Ping Yan[1]; Jeffery R. Whiteaker[1]; Julia Voytovich[1]; Travis Lorentzen[1]; Regine Schoenherr[1]; Amanda G. Paulovich[1]; Pei Wang[2]; *[1]Fred Hutchinson CRC, Seattle , WA; [2]Icahn Institute for Genomics and Multiscale Biology, New York, NY*

MP 704 **A Systems Toxicology Approach to Predict Disease-Like Phenotypes in Human Lung Tissue Models**; Joseph Caruso[1]; Paul Stemmer[1]; *[1]Institute of Environmental Health Sciences, Wayne State University, Detroit, MI*

MP 705 **A Label-Free Informatics Framework for Automated Top-Down Proteoform Relationship Determination and Protein Identification across Multidimensional Chromatographic Space**; Steven Patrie[1]; Casey E Wing[1]; John R Corbett[1]; William S Phipps[1]; Daniel A Plymire[1]; *[1]UT Southwestern Med. Center, Dallas, TX*

MP 706 **Mass-Spectrometry of Single Mammalian Cells Quantifies Proteome Heterogeneity during Cell Differentiation**; Bogdan Budnik[1]; Ezra Levy[2]; Harrison Specht[2]; Nikolai Slavov[3]; *[1]Harvard University, Cambridge, MA; [2]Northeastern University , Boston, MA; [3]Northeastern University, Boston, MA*

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MP 707 **An Ultrafast, Dilute and Shoot-Flow Injection/ MRM method for Quantification of Phenobarbital and Ethyl-D-Glucuronide (EtG) in Urine**; Ravali Alagandula; *Cleveland State University, Cleveland, OH*

MP 708 **Determination of cis-Permethrin, Trans-Permethrin in Rat Plasma and Brain using Gas Chromatography–Negative Chemical Ionization Mass Spectrometry**; Shirin Hooshfar[1]; Darren Gullick[1]; Michael Linzey[1]; Tanzir Mortuza[1]; James V. Bruckner[1]; Catherine A. White[1]; Michael G. Bartlett[1]; *[1]Department of Pharmaceutical and Biomedical Sciences, College of Pharmacy, The University of Georgia, Athens, GA*

MP 709 **Development of multi-Residue LC-MS/MS Method for Determination of Mycotoxins in Animal Feed**; Renat Selimov[1]; Pavel Metalnikov[2]; Alexander Komarov[2]; *[1]VGNKI, Moscow, Russia; [2]VGNKI, Moscow, Moscow*

MP 710 **Development of an Analytical Method for 2,2'-Dimorpholinodiethyl Ether (DMDEE), in Rat Plasma, Amniotic Fluid, and Fetus Homogenate by UPLC-MS/MS**; Teruyo Uenoyama[1]; Melanie A. Rehder Silinski[1]; Reshan A. Fernando[1]; Veronica G. Robinson[2]; Georgia K. Roberts[2]; Suramya Waidyanatha[2]; *[1]RTI International, Research Triangle Park , NC; [2]Division of National Toxicology Program, NIEHS, Research Triangle Park, NC*

MP 711 **Combined Screening and Quantitative Confirmation of 110 Drugs in Urine by LDTD-MS/MS Using a Generic SPE Procedure**; John D. Laycock[1]; Serge Auger[2]; Pierre Picard[2]; Philip Dimson[1]; Karsten Liegmann[1]; David Hall[1]; Jean Lacoursiere[2]; *[1]Tecan-SP, Baldwin Park, CA; [2]Phytronix Technologies, Québec, QC, Canada*

MP 712 **Point-of-Care Identification of Ingested Household Pesticides in Gastric Lavage Content by Laser Desorption-Electrospray Ionization Mass Spectrometry in the Emergency Department**; Chi-Wei Lee[1]; Hung Su[2]; Yang-Kuang Pan[2]; Jentaie Shiea [2]; *[1]Kaohsiung Medical University, Kaohsiung, Taiwan; [2]National Sun Yat-Sen University, Kaohsiung, Taiwan*

MP 713 **Toxicological Screening for over 1000 Compounds in an MRM Based Acquisition for Library ID in Whole Blood Samples**; Alan Barnes[1]; Tiphaine Robin[2]; Sylvain Dulaurent[2]; Souleiman Elbalkhi[2]; Stéphane Moreau[3]; Neil Loftus[1]; Pierre Marquet[2]; Franck Saint-Marcoux[2]; *[1]Shimadzu Corporation, Manchester, UK; [2]CHU Limoges, Limoges, France; [3]Shimadzu Europa GmbH, Duisburg, Germany*

MP 714 **Automatic, Simultaneous and Rapid Analysis of 22 Drugs of Abuse in Saliva by on Line SPE and UHPLC-MS/MS.**; Toinon Doriane[1]; Jaffuel Aurore[2]; Huteau Alban[2]; *[1]Shimadzu, Noisiel; [2]Shimadzu France, Paris, France*

MP 715 **Analysis of the Chemical Warfare Agent VX Isomers in Guinea Pig Blood Following an IV Exposure Utilizing Normal Phase LC-MS/MS**; Christopher E Byers[1]; Michael W Busch[2]; Paul S Demond[2]; Linnzi K. Wright[1]; Ronald A Evans[1]; *[1]US Army ECBC, Aberdeen Proving Ground, MD; [2]Excet, Inc., Springfield, VA*

MP 716 **Analysis of Genital Abnormalities Induced by Fetal Exposure to Endocrine Disrupting Chemicals via Shotgun Proteomics**; Tara Nash[1]; Ciro M Amato[2]; Josua Mogus[2]; Krista McCoy[2]; Michael S Bereman[1]; *[1]North Carolina State University, Raleigh, NC; [2]East Carolina University, Greenville, NC*

MP 717 **Comparison of Genetic and Environmental Mechanisms of Motor Neuron Death by Contemporary Proteomics**; Joshua Beri[1]; Tara Nash[1]; Micheal Bereman[1]; *[1]North Carolina State University, Raleigh, NC*

MP 718 **Data Dependent or Data Independent Acquisition: Evaluation of SWATH for Clinical and Forensic Drug Screening**; Kara L. Lynch[1]; Jeffrey D. Whitman[1]; *[1]University of California, San Francisco, San Francisco, CA*

MP 719 **Elucidation of the Epiproteomic Landscape at the Arsenic Response Locus in S. cerevisiaeby CRISPR-ChAP-MS**; Kirk L West[1]; Zachary J Waldrip[2]; Stephanie Byrum[2]; Ricky D Edmondson[2]; Sam G Mackintosh[2]; Sean D Taverna[3]; Alan J Tackett[2]; *[1]Univ. of Arkansas for Medical Sciences, Little Rock, AR; [2]UAMS, Little Rock, AR; [3]Johns Hopkins School of Medicine, Baltimore , MD*

MP 720 **Investigation of Saliva as an Alternative Matrix for General Unknown Screening of Drugs of Abuse and Medication**; Michael Boettcher[1]; Markus Meyer[2]; *[1]MVZ Labor Dessau GmbH, Dessau-Rosslau, Germany; [2]Bruker Daltonik GmbH, Bremen, Germany*

MP 721 **Quantitative Clinical Toxicological Screening Comparing Library ID from Product Ion Scan MS/MS to MRM Spectrum Mode ID**; Alan Barnes[1]; Tiphaine Robin[2]; Sylvain Dulaurent[2]; Souleiman Elbalkhi[2]; Neil Loftus[1]; Pierre Marquet[2]; Franck Saint-Marcoux[2]; *[1]Shimadzu Corporation, Manchester, UK; [2]CHU Limoges, Limoges, France*

AMBIENT IONIZATION: APPLICATIONS I
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TP 001 ***in situ* Mass Spectrometry for Chemical Identification of Live Cells with Milliseconds Level Ultrafast Electrophoresis**; Guangming Huang[1]; Hongying Zhu[1]; Gongyu Li[1]; *[1]USTC, Hefei, Anhui*

TP 002 **Screening of Skin Lightening Products for the Corticosteroid Clobetasol Propionate using Direct Analysis in Real Time (DART) and Mass Detection** ; Marian Twohig[1]; Oliver Burt[2]; Chris Stumpf[1]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK*

TP 003 **Ultra-fast Screening of Pesticides in Foods and Agricultural Products with Desorption Corona Beam Ionization (DCBI) Tandem Mass Spectrometry**; Jing Dong[1]; Satoshi Yamaki [2]; Yuki Hashi[3]; Naoki Hamada[1]; *[1]Shimadzu China, Beijing, China; [2]Shimadzu Corporation, Kanagawa, Japan; [3]Shimadzu China, Shanghai, China*

TP 004 **Open Probe Fast GC-MS for Medical Diagnostics and Drug Pills Real Time Analysis**; Uri Keshet[1]; Ramesh Bokka[1]; Alexander B. Fialkov[1]; Tal Alon[1]; Aviv Amirav[1]; *[1]Tel Aviv University, Tel Aviv, Israel*

TP 005 **A Novel Universal and Direct SPME-MS Interface Based on Capillary APPI for Simultaneous Quantitation of Polar and Nonpolar Compounds**; Mario Francesco Mirabelli[1]; Renato Zenobi[1]; *[1]ETH Zurich, Zurich, ZH*

TP 006 **Cleavable Isobaric Peptides as Mass Reporters for Mass Spectrometry-based Immunoassays**; Tatiana Vélez-Burgos[1]; Jay Kim[1]; Yosef Maher[1]; Abraham K. Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

TP 007 **Detection and Quantification of Atomic Ions with Flowing Atmospheric-Pressure Afterglow Mass Spectrometry**; Garett M. MacLean[1]; Jacob T. Shelley[1]; *[1]Rensselaer Polytechnic Institute, Troy, New York*

TP 008 **Extractive Atmospheric Pressure Photoionization (EAPPI) Mass Spectrometry: Rapid Analysis of Chemicals in Complex Matrices**; chengyuan liu[1]; Yang Pan[1]; *[1]University of Science and Technology of China, Hefei, China*

TP 009 **Molecular Characterization of Exhaust Particulate Matters Using Internal Extractive Electrospray IonizationMass Spectrometry**; Hua Zhang[1, 2]; Yi Li[2]; Liang Zhu[2]; Huanwen Chen[2]; *[1]State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of Chemistry, Jilin University, Changchun, China; [2]East China University of Technology, Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, Nanchang, China*

TP 010 **Rapid Classification of Medulloblastoma Subgroups for Optimal Treatment Planning Using a Hand Held Cold Laser Ablation Mass Spectrometry Probe**; Michael Woolman[1]; Jing Zou[1]; Megan Wu[2]; Semra Isik[2]; Claudia M Kuzan-Fischer[2]; Isabelle Ferry[2]; Sunit Das[2]; Michael D Taylor[2]; James T Rutka[2]; Howard Ginsberg[1]; Arash Zarrine-Afsar[3]; *[1]University of Toronto, Toronto, ON; [2]Hospital for Sick Children, Toronto, Ontario; [3]Toronto, ON*

TP 011 **Rapid Molecular Analysis and Comparison of Canine, Feline and Human Tumour Samples with REIMS; Metastasis based Identification of Primary Tumour**; Julia Balog[1, 2]; Richard Schaffer[1]; Steven Derek Pringle[2, 3]; Zoltan Takats[2]; *[1]Waters Research Center, Budapest; [2]Imperial College London, London; [3]Waters Corporation, Manchester*

TP 012 **Thermal Desorption Combined with Flame Atmospheric Pressure Chemical Ionization Mass Spectrometry to Rapidly Determine Chemical Compounds**; Hung Su[1]; Shih-Hsi Chen[1]; Sy-Chyi Cheng[1]; Jentaie Shiea [1]; *[1]National Sun Yat-Sen University, Kaohsiung, Taiwan*

TP 013 **Utilizing Solid Phase Extraction Technologies to Facilitate DART-basedHigh-ThroughputAmbient Ionization-MS Analysis of Biological Samples**; Brian D. Musselman [1]; Fredrick Li[1]; Joseph Tice[1]; *[1]IonSense, Inc., Saugus , MA*

TP 014 **A Comparative Study of Nitrogen Versus Helium Direct Analysis in Real Time Mass Spectrometry for the Analysis of Polar Compounds**; Liguo Song[1]; Wei Chean Chuah[1]; Edward Remsen[2]; John E Bartmess[3]; *[1]Western Illinois University, Macomb, IL; [2]Bradley University, Peoria, IL; [3]University of Tennessee, Knoxville, TN*

TP 015 **Analysis of Degraded Polybutylene Terephthalate (PBT) Products by Thermal Desorption and Pyrolysis Combined with DART-MS (TDP/DART-MS)**; Chikako Takei[1]; Yasuyuki Semba[1]; Kenichi Yoshizawa[1]; *[1]BioChromato, Inc., Fujisawa, Japan*

TP 016 **Analysis of Macrolides Antibiotics by Direct Analysis in Real-Time Mass Spectrometry with Glycerin as Dopant**; Qing Yang[1]; Jiyuan Guo[1]; Bin Xu[2]; Weihong Zhang[2]; Xiaokun Duan[2]; Charles C. Liu[2]; *[1]Department of Quality Inspection, New Hope Liuhe Co., Ltd, Qingdao, China; [2]ASPEC Technologies LTD, Beijing, China*

TP 017 **Analysis of Tea Aroma by Direct Analysis in Real-Time Mass Spectrometry**; Li Zhang[1]; Bin Xu[2]; Xiaokun Duan[2]; Charles C. Liu[2]; *[1]Suzhou Vocational University, Suzhou, China; [2]ASPEC Technologies LTD, Beijing, China*

TP 018 **Analysis of Weakly Interacting Dicopper Formamidinate Complexes by Direct Analysis in Real Time (DART) Mass Spectrometry**; Michael Pastor[1]; O. David Sparkman[1]; Qinliang Zhao[1]; *[1]University of the Pacific,*

Stockton, California

TP 019 **Chemotaxonomy of Astyanax and Drosophila by DART-MS Analysis of fatty acids and Ozonolysis-Derived Fatty Acyl Fragments**; Joanne Y. Yew[1]; Masato Yoshizawa[2]; Robert B. Cody[3]; *[1]Pacific Biosciences Research Center, University of Hawaii at Manoa, Honolulu, HI; [2]Department of Biology, University of Hawaii at Manoa, Honolulu, HI; [3]JEOL USA Inc., Peabody, MA*

TP 020 **Comparison of Portable near-IR and Laboratory mid-IR Sources for Laser Ablation Atmospheric Pressure Photoionization MS**; Raveendra C. Wickramasinghe[1]; Yeni P. Yung[1]; Anu Vaikkinen[2]; Tiina J. Kauppila[2]; Luke Hanley[1]; *[1]University of Illinois at Chicago, Chicago, IL; [2]University of Helsinki, Helsinki, Finland*

TP 021 **Dark Discharge Assisted Direct Analysis in Real Time Ionization using Argon**; Motoshi Sakakura[1]; Teruhisa Shiota[1]; Mitsuo Takayama[2]; Kanako Sekimoto[2, 3]; *[1]AMR Inc., Meguro-ku, Japan; [2]Yokohama City Univ., Yokohama, Japan; [3]NOAA Earth System Research Laboratory, Boulder, CO*

TP 022 **MS/MS Applications of the iKnife in Breast Surgery: Towards Triple-Quadrupole Based Real-Time Tissue Identification**; Zsolt Bodai[1]; Edward St John[1]; Emma White[1]; April Covington[1]; James McKenzie[1]; Francesca Rosini[1]; Hui-Yu Ho[1]; Julia Balog[2]; Daniel Leff[1]; Zoltan Takats[1]; *[1]Imperial College London, London; [2]Waters Research Center, Budapest*

TP 023 **Rapid Detection of Explosives using Thermal Desorption DART-MS and Reverse Library Search**; Frederick Li[1]; Joseph Tice[1]; Stephen Shrader[2]; Brian Musselman[1]; *[1]IonSense Inc., Saugus, MA; [2]Shrader Software Solutions, Grosse Pointe Park, MI*

TP 024 **Rapid Screening of Explosives in Ambient Environment by Aerodynamic Assisted Thermo Desorption Mass Spectrometry**; Jianli Liu[1]; Qiang Zhao[1]; Wei Xu[1]; *[1]Beijing Institute of Technology, Beijing, China*

TP 025 **Real-Time Organic Aerosol Analysis via Vacuum-assisted Plasma Ionization (VaPI) Ion Mobility-Mass Spectrometry.**; Sandra L. Blair[1]; Stephen C. Zambrzycki[1]; Anyin Li[1]; Masayuki Takeuchi[1]; Charles L. Liotta[1]; Nga L. Ng[1]; Facundo M. Fernández[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

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TP 026 **Elimination of ADE-induced Dengue Virus Infection by a Novel Reagent DCAF**; Shan Feng; *Tsinghua University, Beijing, Beijing; University of Notre Dame, Notre Dame, IN*

TP 027 **Investigating Product Quality of HIV Monoclonal Antibody by LC-MS Analysis**; Vera B. Ivleva[1]; Nicole A. Schneck[1]; Q. Paula Lei[1]; K. C. Cheng[1]; *[1]NIH/NIAID/VPPL, Gaithersburg, MD*

TP 028 **Evaluation of Protein Aggregation in Biopharmaceutical using Chemical Cross-linking MS and Quantitative Laser diffraction**; Yuzo Yamazaki[1]; Kenji Saito[2]; Hiroki Maeda[1]; Yuji Shoya[2]; Masayoshi Toyoura[2]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Biomedical R&D Department, Pharma Foods International, Japan*

TP 029 **Factors Affecting Spectral Quality of Monoclonal Antibodies from Time-of-Flight Mass Spectrometers**; Jeff Brown[1]; Jonathan Williams[1]; Emmy Hoyes[1]; Dale Cooper-Shepherd[1]; Francesco Lanucara[1]; Laetitia Denbigh[1]; Michael Morris[1]; *[1]Waters Corporation, Wilmslow, UK*

TP 030 **Characterization of a Cysteine-conjugated ADC on a Hybrid Quadrupole-Orbitrap Mass Spectrometer**; Xiaoxi Zhang[1]; Jun Lin[2]; *[1]ThermoFisher Scientific, Shanghai, China; [2]Genor Biopharma Co., Ltd., Shanghai, China*

TP 031 **Characterizing and Quantitating Therapeutic Antibody and Drug Conjugate Biotransformation using High Throughput On-Tip Affinity Capture Mass Spectrometry**; John C. Tran[1]; Ke Sherry li[2]; Jianyong Wang[2]; Phillip Y Chu[2]; Aimee Fourie[2]; Robert Tchelepi[2]; Katherine R Kozak[2]; Yichin Liu[2]; *[1]Genentech, South San Francisco, CA; [2]Genentech, Inc, South San Francisco, CA*

TP 032 **Qualitative Analysis of Antibody-Drug Conjugates (ADCs): An Experimental Evaluation of Common Analytical Techniques for Direct Comparison**; Malin Källsten[1, 2]; Rafael Hartmann[1, 2]; Konstantin Artemenko[1]; Fredrik Lehmann[2]; Jonas Bergquist[1]; *[1]Uppsala University, Uppsala, Sweden; [2]Recipharm OT Chemistry AB, Uppsala, Sweden*

TP 033 **Understanding the Limits of Quantitation for Intact Proteins using Microfluidic LC-MS**; Gregory Roman[1]; James Murphy[1]; *[1]Waters Corp, Milford, MA*

TP 034 **Comprehensive Characterization on Monoclonal Antibody using a Newly Developed Q-TOF/MS Instrument**; David Wong[1]; Jing Chen[2]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]Agilent Technologies, Inc., Madison, WI*

TP 035 **Gas-phaserearrangement byClDof Calicheamicin-based LP with Cleavable Linker Containing Aminobenzylcarbamate Group**; Xidong Feng[1]; Dahui Zhou[1]; Kenneth Dirico[1]; Russell Dushin[1]; Chakrapani Subramanyam[1]; Christopher J O'Donnell[1]; *[1]Pfizer, Groton, CT*

TP 036 **Development of Native and Denaturing LC-MS Methods for Characterization of Cysteine-Linked Antibody Drug Conjugates Using a Non-Toxic Mimic**; Kevin Ray[1]; Nicolas Caffarelli[1]; Gordon NicoL[1]; Ben Cutak[1]; Brian Gau[1]; Jeff Turner[1]; *[1]MilliporeSigma, St. Louis, MO*

TP 037 **Hybrid-MS Analyses of IgG1 Antibodies: Confirmation of Conformation**; Rosie Upton[1]; Kamila J Pacholarz[1]; Lukasz Migas[1]; Amy Campbell[2]; Perdita E Barran[1]; David Firth[3]; *[1]University of Manchester, Manchester, UK; [2]University of Liverpool, Liverpool, Merseyside; [3]Covance Laboratories Ltd., Harrogate, UK*

TP 038 **Native Ion Mobility Mass Spectrometry for the Characterization of Biotherapeutics**; Dale A. Cooper-Shepherd[1]; Jakub Ujma[1]; Kevin Giles[1]; Laetitia F. Denbigh[1]; Nick Tomczyk[1]; *[1]Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK*

TP 039 **Insights from Native Mass Spectrometry Approaches for Top- and Middle- Level Characterization of Site-Specific Antibody-Drug Conjugates**; Thomas Botzanowski[1]; Stephane Erb[1]; Oscar Hernandez Alba[1]; Anthony Ehkirch[1]; Olivier Colas[2]; Elsa Wagner-Rousset[2]; David Rabuka[3]; Penelope Drake[3]; Alain Beck[2]; Sarah Cianferani[1]; *[1]Laboratoire de Spectrométrie de Masse BioOrganique, University of Strasbourg, Strasbourg, France; [2]Centre d'Immunologie Pierre-Fabre, Saint-Julien-en-Genevois, France; [3]Catalent Biologics West, Emeryville, CA*

TP 040 **Characterizing Trastuzumab-Drug Conjugates by High Resolution Native Mass Spectrometry, Ion Mobility, and Molecular Dynamics Simulations**; Liuqing Shi[1]; Bernadette V. Marquez-Nostra[2]; Suzanne E. Lapi[3]; Weidong Cui[4]; Michael L. Gross[1]; *[1]Washington University, St Louis, MO; [2]Washington University School of Medicine, St. Louis, MO; [3]University of Alabama at Birmingham, Birmingham, AL; [4]Washington University, St. Louis , MO*

TP 041 **Higher Order Structural Analysis of Biotherapeutics Exposed to Sample Handling Stress Conditions**; Richard A Kerr[1]; Hongping Ye[1]; *[1]FDA Department of Pharmaceutical Analysis, St Louis, MO*

TP 042 **Intact Mass Analysis and DAR Calculation for Antibody-Drug Conjugates**; Marshall W. Bern[1]; Yong J. Kil[1]; Eric Carlson[1]; K. Ilker Sen[1]; St John Skilton[1]; Michael Peddicord[2]; Wei Ding[2]; *[1]Protein Metrics Inc., San Carlos, CA; [2]Bristol-Myers Squibb, New Brunswick, NJ*

TP 043 **Evaluation of an ADC's DAR in Rat Serum by Affinity**

Capture and Mass Spectrometry; Maria Christina Malinao[1]; Cody A Warhurst[1]; Julien Dugal-Tessier[1]; Josh T. Snyder[1]; Brian A Mendelsohn[1]; *[1]Agensys, Inc., Santa Monica, CA*

TP 044 **How to Tailor Holistic Analytical Solutions for Therapeutic Bioconjugates to Reveal Previously Unknown Conjugatable Modifications**; Wesley Zmolek[1]; Qiuting Hong[1]; William E Haskins[1]; *[1]Redwood Bioscience (Catalent Biologics-West), Emeryville, CA*

TP 045 **A Mass Spectrometric Method for Readily Identifying Peptides Modified with vcMMAE in Antibody-Drug Conjugate Enzyme Digests**; Ioannis A Papayannopoulos[1]; Shannon Renn-Bingham[1]; Jarrod M Womble[1]; *[1]Celldex Therapeutics, Inc., Fall River, MA*

TP 046 **Analysis of Monoclonal Antibodies in Human Serum for Monoclonal Gammopathy Diagnosis by 21 Tesla FT-ICR Top-Down and Middle-Down MS/MS**; Lidong He[1]; Lissa Anderson[2]; David R. Barnidge[3]; David L. Murray[3]; Christopher L Hendrickson[1, 2]; Alan G. Marshall[1, 2]; *[1]Florida State University, Tallahassee, Florida; [2]National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; [3]Mayo Clinic, Rochester, MN*

TP 047 **Kinetics of Intracellular Dolastatin Accumulation in EGFR Expressing Cell Lines after Antibody-drug Conjugate Dosing**; Ken Durbin; *AbbVie, North Chicago, IL*

TP 048 **De-conjugation Coupled with LC-MS for Investigating the Stability of Small Molecule Drugs in Antibody-Drug Conjugates**; Tao Chen[1]; Dian Su[1]; Jason Gruenhagen[1]; Yi Li[1]; Peter Yehl[1]; Nik Chetwyn[1]; Colin Medley[1]; *[1]Genentech, Inc., South San Francisco, CA*

TP 049 **Application of ETD to the Characterization of ADC Product Attributes That Are Challenging to the Traditional Approach**; Zhiqi Hao[1]; Qiuting Hong[2, 3]; Michael Kim[1]; Diana Liu[1]; William Haskins[1, 3]; Yan Chen[1]; *[1]Genentech, Inc, South San Francisco, CA; [2]Eurofins Lancaster Laboratories, Inc., Lancaster, PA; [3]Catalent Pharma Solutions, Emeryville, CA*

TP 050 **Characterization of a Degradation Product of an IgG1 Monoclonal Antibody by Tandem Mass Spectrometry and Other Biophysical Techniques**; Ekaterina G. Deyanova[1]; Yun Wang[2]; Yuan Cheng[2]; Jun Dai[2]; Brent Meengs[3]; Jason Chen[2]; Jonathan Wert[3]; Yingru Zhang[2]; Olafur Gudmundsson[2]; Susan Julien[3]; Guodong Chen[2]; *[1]Bristol-Myers Squibb, Princeton, NJ; [2]Bristol-Myers Squibb, Princeton, NJ; [3]Bristol-Myers Squibb, Seattle, WA*

TP 051 **A Direct Comparison of Top-Down and Bottom-Up HDX-MS for Antibody Characterization**; Jingxi Pan[1, 2]; Suping Zhang[3]; Christoph H. Borchers[1, 4]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC; [2]Division of Medical Sciences, University of Victoria, Victoria, BC; [3]MRM Proteomics, Victoria, BC; [4]Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC*

TP 052 **Antibody Sequence Validation by Peptide and Disulfide Bridge Mapping**; Yi Liu[1]; Lei Xin[2]; Baozhen Shan[2]; Kaizhong Zhang[1]; *[1]University of Western Ontario, London, ON; [2]Bioinformatics Solutions Inc, Waterloo, ON*

TP 053 **ImmunocaptureLC-HRMS for the Quantitation of Therapeutic Monoclonal Antibody Ipilimumab Using Light Chain Approach**; Yongxin Zhu[1]; John Mehl[1]; France Landry[1]; Srikanth Kotapati[2]; David Passmore[2]; Haiqing Wang[1]; Eugene Ciccimaro Jr.[1]; Timothy Olah[1]; *[1]Bristol-Myers Squibb, Princeton, NJ; [2]Bristol-Myers Squibb, Redwood City, CA*

TP 054 **Quantitative HPLC-MS/MS Analysis of DM1 and DM1-MCC Extracted from Whole Blood Dried onto a Mitra Microsampling Device**; Chad D. Christianson[1]; Michael D. Williams[1]; Natalie C. Garcia[2]; Katherine M. Yahvah[1]; *[1]Alturas Analytics, Moscow, ID; [2]Neoteryx, LLC, Torrance, CA*

TP 055 **High-Resolution Accurate-Mass LC-MS enables In-Depth Characterization of *in vivo* Biotransformations for Intact Antibody-Drug Conjugates**; Jintang He[1]; Dian Su[1]; Carl Ng[1]; Luna Liu[1]; Shang-Fan Yu[1]; Thomas Pillow[1]; Geoffrey Del Rosario[1]; Surinder Kaur[1]; Keyang Xu[1]; *[1]Genentech, Inc, South San Francisco, CA*

TP 056 **Application of Non-Reduced Peptide Mapping by Mass Spectrometry (MS) for the Characterization of Site-Specific Cysteine Antibody-Drug Conjugates**; Andrew W. Dawdy[1]; Jason C. Rouse[2]; Olga V. Friese[1]; *[1]Pfizer Inc, St Louis, MO; [2]Pfizer Inc., Andover, MA*

TP 057 **Assessing Biosimilarity of Eight Different Batches of Commercial Herceptin with Similarity Index Derived from Comprehensive Biophysical Data**; Mowei Zhou[1]; Alejandro Heredia-Langner[1]; David Bush[2]; Erika Zink[1]; Xueyun Y Zheng[1]; Ernesto Nakayasu[1]; Erin S Baker[1]; Charles Ansong[1]; John Cort[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Genedata, Lexington, MA*

TP 058 **Evaluation of Factors Affecting Detection of Host Cell Proteins in Biotherapeutic Proteins using an Orbitrap Fusion Lumos Tribrid Mass Spectrometer**; Stephane Houel[1]; Michael Blank[1]; Romain Huguet[1]; Seema Sharma[1]; Martin Samonig[2]; Vlad Zabrouskov[1]; Jonathan Josephs[1]; *[1]Thermo Fisher Scientific, San Jose, California; [2]Thermo Fisher Scientific, Bremen, Germany*

TP 059 **Highly Automated Analysis of Antibody Chain Shuffling in Bispecific Antibodies**; Marshall Bern[1]; Yong J. Kil[1]; Eric Carlson[1]; Brian D. Soriano[2]; Stone D.-H. Shi[2]; *[1]Protein Metrics Inc., San Carlos, CA; [2]Amgen, Thousand Oaks, CA*

TP 060 **Full Validation of Therapeutic Antibody Sequences by Middle-Up Mass Measurements and Middle-Down Protein Sequencing as a Routine Task**; Anja Resemann[1]; Wolfgang Jabs[2]; Elsa Wagner[3]; Olivier Colas[3]; Waltraud Evers[1]; Jason S. Wood[4]; Eckhard Belau[1]; Lars Vorwerg[1]; Alain Beck[3]; Detlev Suckau[1]; *[1]Bruker Daltonics, Bremen, Germany; [2]Beuth University of Applied Sciences Berlin, Berlin, Germany; [3]Laboratories Pierre Fabre, Paris, France; [4]Bruker Daltonics, Billerica, MA*

TP 061 **Pilot Study Regarding Automated Comparative Fd- and Fc-Domain MS-Based Glycoprofiling for High-Throughput Online Process Monitoring of Therapeutic Antibody Production**; Sven Bahrke[1]; Robert Wilmanowski[1]; Martin Hedström[2]; Dag Erlandsson[2]; Fredrik Olsson[2]; Detlev Suckau[3]; Wolfgang Jabs[4]; *[1]Glycotope GmbH, Berlin, Germany; [2]CapSenze Biosystems AB, Lund, Sweden; [3]Bruker Daltonik GmbH, Bremen, Germany; [4]Beuth University of Applied Sciences Berlin, Berlin, Germany*

TP 062 **Use Information Independent SWATH Acquisition for Biotherapeutic Peptide Mapping**; Ji Luo; *Shanghai AB Sciex Analytical Instrument Trading Co., Ltd, Shanghai, China*

TP 063 **BiopharmaViewTM Software as a Robust Tool for Automated Quantitation of Oxidation Sites in Monoclonal Antibody Characterization**; Kerstin Pohl[1]; Annu Uppal[2]; Amandine Boudreau[3]; *[1]SCIEX, Darmstadt, Germany; [2]SCIEX, Gurgaon, India; [3]SCIEX, Concord, ON*

TP 064 **Rapid Method for IgG Met-255 Oxidation Level Determination by LC-MS. Method Development and Qualification**; Tomasz Welerowicz[1]; Tomasz Gozdziewicz[1]; Radoslaw Obuchowicz[1]; Marianna Sztolpa[1]; Krystian Siten[1]; Pawel Socha[1]; Michael Safinowski[1]; Piotr Zien[1]; *[1]Polpharma Biologics, Gdansk, Poland*

TP 065 **HRAMS Monitoring of *in-vivo* Protein Biotransformation's: Quantitative Determination of Trastuzumab and Deamidation Products in Human Plasma by MRMHR and SWATH®**; Jason Causon[1]; Kees Bronsema[2]; Nico Van De Merbel[2]; Peter Bults[2]; Edwin Hooijschuur[2]; Martijn Hilhorst[2]; Milla Neffling[1]; Neil Walsh[1]; *[1]SCIEX, Warrington, Cheshire; [2]PRA HealthSciences, Assen, Netherlands*

TP 066 **Antibody Verification by Protein Immunoprecipitation**

and Mass Spectrometry (IP-MS) Characterizes Antibody Performance and Identifies Protein-Protein Interactions; Gregory K. Potts[1]; Bhavin Patel[1]; Leigh Foster[1]; John C. Rogers[1]; *[1]Thermo Fisher Scientific, Rockford, IL*

TP 067 **Controlled, In-membrane Protein Digestion for Antibody Characterization and Assessment of Structural Changes**; Merlin Bruening[1]; Yongle Pang[2]; Weijing Liu[1]; Wenjing Ning[2]; Nitin Patel[3]; Gia Jokhadze[3]; *[1]University of Notre Dame, Notre Dame, IN; [2]Michigan State University, East Lansing, MI; [3]Takara Bio, Mountain View, CA*

TP 068 **Evaluation of a Microfluidic Electrophoresis Device Coupled to an Orbitrap Mass Spectrometer for the Characterization of Biotherapeutics Proteins**; Stephane Houel[1]; Erin Redman[2]; Scott Mellors[2]; Aaron Bailey[1]; Chris Petty[3]; Aran Paulus[1]; Kai Zhou[4]; Jonathan Josephs[1]; *[1]Thermo Fisher Scientific, San Jose, California; [2]908 Devices, Inc., Carrboro, NC; [3]908 Devices Inc., Boston, MA; [4]Thermo Fisher Scientific, Cambridge, MA*

TP 069 **Evaluation of the Arginine Specific Protease RgpB for LC-MS Based Antibody Analysis**; Sheila Maibom-Thomsen[1, 2]; Peter Højrup[2]; Jakob Bunkenborg[1]; Malin Mejare[3]; Ejvind Mørtz[1]; Fredrik Olsson[3]; Thomas Kofoed[1]; Maria Nordgren[3]; *[1]Alphalyse, Odense, Fyn; [2]University of Southern Denmark, Odense, Denmark; [3]Genovis, Lund, Sweden*

TP 070 **Physicochemical Characterization of an Original and Biosimilar Omalizumab by Mass Spectrometry Methods**; Maksim Degterev[1]; Rakhim Shukurov[1]; Alexander Vishnevskiy[1]; Igor Fabrichniy[1]; *[1]IBC Generium, Vol'ginskiy*

TP 071 **Mass Spectrometry as an Orthogonal Technique to Quality Control and Sequencing in Recombinant mAb Production**; Scott A Robotham[1]; Jason Hogan[2]; Nicole Bracy-Johson[1]; Holly Palme[1]; Aarti Jashnani[2]; Jia Dong[2]; Billy Akinsanya[1]; Adela Buzescu[1]; Andy Deng[2]; Meaghan Happer[2]; Jonathan R Haulenbeek[1]; *[1]Bristol-Myers Squibb, Princeton, NJ; [2]Bristol-Myers Squibb, Redwood City, CA*

TP 072 **Establishing Translation of a Whole-Molecule LC-MS Assay for *in vivo* Quantitation of mAbs: From Pharmacokinetic Analyses to Critical Quality Attributes**; John F. Kellie[1]; Robert A. Biddlecombe[2]; Sarah Childs[2]; Molly Z. Karlinsey[1]; *[1]GSK, King of Prussia, PA; [2]GSK, Stevenage, UK*

TP 073 **Mapping the Effects of UV Irradiation on Monoclonal Antibody Drugs**; J. Larry CampbelL[1]; Chris Lock[1]; Brendon Seale[2, 3]; J.C. Yves Leblanc[2]; Suya Liu[2]; Xu Guo[2]; Wen Jin[2]; Michael Sasges[4]; Michelle Gabriel[4]; Mark Schofield[5]; Marc Aucoin[6]; Emma Dare[6]; *[1]SCIEX, Concord, ON; [2]SCIEX, Concord, ON, ON; [3]University of Toronto, Toronto, ON; [4]Trojan Technologies, London, Ontario; [5]Pall Corporation, Westborough, MA; [6]University of Waterloo, Waterloo, Ontario*

TP 074 **Characterization of N-glycans in Therapeutic Glycoproteinsby Hydrophilic Interaction Ultra High Performance Liquid Chromatography-Fluorescence-Mass Spectrometry (HILIC-UHPLC-FLD-MS)**; Annette Vogt[1]; Cornelia Wagner[1]; Babette Werner[1]; Andreas Adlberger[1]; Laurent Lariviere[1]; Hans Koll[1]; *[1]Roche Pharma Research and Early Development (pRED), Large Molecule Research, Roche Innovation Center Munich, Penzberg, Germany*

TP 075 **Comparative Fc N-glycosylation Profiling at Glycopeptide Level for Differentiation and Verification of Monoclonal Antibody Therapeutics using HILIC-SPE Coupled to MALDI-TOF-MS**; Lianji Jin; *FDA, Cincinnati, OH*

TP 076 **Degradation Study of the NISTmab Reference Material: From the Discovery to Routine Quantification of Stress Related Artefacts**; Guillaume Tremintin[1]; Detlev Suckau[2]; Peter Hufnagel[2]; *[1]Bruker Daltonics, Fremont, CA; [2]Bruker Daltonik GmbH, Bremen, Germany*

TP 077 **Multilevel Characterisation of Site-Specific Antibody Drug Conjugates (ADC) using RP-UPLC-ESI-MS** ; Sylwia Jozwiak[1]; James Graham[1]; *[1]Lonza Biologics, Slough, Berkshire*

TP 078 **Determination of Released Payload Species of Antibody Drug Conjugates with Noncleavable Linkers by High Resolution Mass Spectrometry and MetabolitePilot Software**; Ian Moore[1]; Yuan-Qing Xia[2]; *[1]SCIEX, Concord, ON; [2]Sciex, Framingham, MA*

TP 079 **Routine Host Cell Protein (HCPs) Monitoring and Non-Targeted New Feature Detection and Identification as Part of Mass Spectrometry-based Quality Control** ; Michael Blank[1]; Stephane Houel[1]; Jonathan Josephs[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

TP 080 **Toward *de novo* Sequencing of Mixtures of Antibodies**; Natalie Castellana[1]; Kexin Huang[2]; Alice Liang[2]; Siyang Wang[2]; Hua Tu[2]; *[1]Digital Proteomics, LLC., La Jolla, CA; [2]LakePharma, Inc., Belmont, CA*

TP 081 **Automatic End-to-End *de novo* Sequencing (Including I/L) of Antibodies with EThcD Fragmentation**; Wilfred H. Tang[1]; Yong J. Kil[1]; K. Ilker Sen[1]; Marshall Bern[1]; Shruti Nayak[2]; Beatrix Ueberheide[2]; Gregg Silverman[2]; *[1]Protein Metrics, San Carlos, CA; [2]New York University Langone Medical Center, New York, NY*

TP 082 **Automated Determination of ADC Drug-Antibody Ratios Using an Open Access System**; Tanner Stevenson[1]; Stephen Madden[2]; David Wong[2]; Jade C. Byrd[2]; Robert Williams[2]; *[1]Agilent Technologies, Santa Clara, CA; [2]Agilent Technologies Inc., Santa Clara, CA*

TP 083 **Practical Glycan Analysis: Comparison of Methods for Characterizing Glycan Profiles of Recombinant Monoclonal Antibodies**; Loredana Serafini[1]; Gregory Staples[2]; Caroline S. Chu[2]; Andy Gieschen[2]; Adele Taylor[3]; Greg Tuffy[1]; Mark Nagel[1]; Cody Williams[4]; Justin Golde[4]; Gregg Czerwieniec[1]; Katherine M. Brendza[1]; Roman Sakowicz[1]; *[1]Gilead Sciences, Foster City, CA; [2]Agilent Technologies, Inc., Santa Clara, CA; [3]ProZyme, Hayward, CA; [4]Hamilton Robotics, Reno, Nevada*

TP 084 **Fast Stability Assessment of a Next Generation Antibody Drug Conjugate by N-Acetylcysteine-Drug Conjugate Model Compound Degradation Study**; Chunang (Christine) Gu[1]; Omar Hamdy[1]; John Peattle[1]; lieza Danan-leon[1]; Tony Cano[1]; *[1]Abbvie Stemcentrx LLC, South San Francisco, CA*

TP 085 **A Novel LC/MS-based Pipeline Enabling Comprehensive Investigation of Tumor/Tissue Disposition of Antibody-Drug-Conjugate, *in vivo* DAR, Free Toxin and Antigen Turnover**; Bo An[1]; Ming Zhang[1]; Yang Qu[1]; Yuan-ju Chen[1]; Jun Qu[1]; *[1]SUNY at Buffalo, Buffalo, NY*

TP 086 **Profiling the N-Glycosylation of Biotherapeutic IgGs with HILIC-MRM Analysis of Trypsin Digested Culture Media**; Ron Orlando[1, 2]; Gerardo Gutierrez[2]; Tyler Fletcher[3]; *[1]University of Georgia, Athens, GA; [2]GlycoScientific, LLC, Athens, GA; [3]University of Georgia, Athens, GA*

TP 087 **Improved Top-Down and Middle-Down Characterization of Antibodies using Multiple Ion Activation Techniques on a Modified Orbitrap Tribrid Mass Spectrometer**; Luca Fornelli[1]; Kristina Srzentić[1]; Romain Huguet[2]; Stephane Houel[2]; Aaron Bailey[2]; Helene Cardasis[2]; Ryan T. Fellers[1]; Tara Schroader[2]; Horn M. David[2]; Seema Sharma[2]; Philip D. Compton[1]; Jonathan Josheph[2]; Vlad Zabrouskov[2]; Mike Senko[2]; Neil L. Kelleher[1]; *[1]Northwestern University-Kelleher Research Group, Evanston, IL; [2]Thermo Fisher Scientific, San Jose, CA*

TP 088 **N-linked Glycan Profiling for Monoclonal Antibodies using Bottom-Up and Middle-Down LC-MS Approaches**; Lin He[1]; Jonathan Krieger[2]; Paul Taylor[2]; Baozhen Shan[1]; *[1]Bioinformatics Solutions Inc, Waterloo, ON; [2]Hospital for Sick Children, Toronto, Ontario*

TP 089 **LC-MS/MS Quantitative Method Development of**

Herceptin Based on nSMOL Technology and Skyline Software; Hongyuan Hao[1]; Qiaoxia Liu[1]; Taohong Huang[1]; *[1]Shimadzu (China) Co.,Ltd., Shanghai*

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TP 091 **Bioanalytical Method Development for the Determination of Desmosine and Isodesmosine in Mouse Urine by ion-pair reverse phase LC-MS/MS**; Philip S. Wong[1]; Jian Jiang[1]; Christopher A James[1]; *[1]Amgen, Thousand Oaks, CA*

TP 092 **Absolute Quantification of Site-Specific Core-Fucosylation of Serum Fibronectin in Alcohol-Related Hepatocellular Carcinoma**; Haidi Yin[1]; David M. Lubman[2]; Zhongping Yao[1]; *[1]The Hong Kong Polytechnic University, Hong Kong, China; [2]University of Michigan, Ann Arbor, MI*

TP 093 **A fast and Sensitive LC-MS/MS Method for the Determination of Lyso-Gb3 in Human Plasma**; Wuyi (Charlie) Zha[1]; Karolina Doda[1]; Mohamed Osman[1]; Xinping Fang[1]; *[1]WuXi AppTec. Inc, Plainsboro Township, NJ*

TP 094 **Quantitative Proteomic Analysis of Serum Exosomes from Patients with locally Advanced Pancreatic Cancer Undergoing Chemoradiotherapy**; Mingrui An[1]; Kyle C. Cuneo[1]; Jianhui Zhu[1]; Jing Wu[1]; Jing Liang[1]; Mengmeng Wang[1]; David M. Lubman[1]; *[1]University of Michigan Medical Center, Ann Arbor, MI*

TP 095 **Quantification Performance of Non-Invasive LC-MS/MS Analysis and Evaluation of Undifferentiated State of Human iPS Cells**; Kenichi Toyoda[1]; Takashi Suzuki[1]; Kunitada Hatabayashi[2]; Kenichi Kagawa[2]; Masatoshi Takahashi[1]; *[1]Shimadzu Corporation, Nakagyo-ku, Japan; [2]Tokyo Electron Limited, Minato-ku, Japan*

TP 096 **Biomarker Monitoring by Quantitative MALDI Imaging: Application to the Tryptophan-Kynurenine Pathway in Immuno-Oncology**; Rima Ait-Belkacem[1]; Vanesa Bol[2]; David Bonnel[1]; Bruno Gomes[2]; Jonathan Stauber[1]; *[1]Imabiotech, Loos, France; [2]iTeos Therapeutics SA, Gosselies, Belgium*

TP 097 **Investigation of Protective Mechanism of a Bacterial Mixture of Human Commensals against Colon Tumorigenesis by Quantitative Proteomics Analysis**; Jing Wu[1]; Mingrui An[1]; Jianhui Zhu[1]; Grace Y. Chen[1]; David M. Lubman[1]; *[1]University of Michigan Medical Center, Ann Arbor, MI*

TP 098 **Verification of Genomics Biomarker Candidates for Prostate Cancer at the Protein Level Using SRM-MS**; Hui Wang[1]; Yuqian Gao[1]; Athena schepmoes[1]; Gyorgy Petrovics[2]; Jennifer Cullen[2]; Thomas Fillmore[1]; Tujin Shi[1]; Wei-Jun Qian[1]; Richard Smith[1]; Brandi Weaver[3]; Robin Leach[3]; Ian Thompson[3]; Sudhir Srivastava[4]; Albert Dobi[2]; Karin Rodland[1]; Jacob Kagan[4]; Shiv Srivastava[2]; Tao Liu[1]; *[1]PNNL, Richland, wa; [2]Uniformed Services University of the Health Sciences, Bethesda, MD; [3]Univerysity of Texas Health and Science Center at San Antonio, San Antonio, TX; [4]National Cancer Institute, Bethesda, MD*

TP 099 **Quantitative Targeted-SIM Assay for Neuron-specific Enolase in Small-cell Lung Cancer using Formalin-fixed Paraffin-embedded Tissue Samples**; Kiyonaga Fujii[1]; Yuka Miyata[2]; Ikuya Takahashi[2]; Hirotaka Koizumi[1]; Hiromasa Tojo[1]; Hisashi Saji[1]; Toshiaki Somehara[1, 2]; Masayuki Takagi[1]; Haruhiko Nakamura[1]; Toshihide Nishimura[1]; *[1]St. Marianna University School of Medicine, Kawasaki, Japan; [2]Nissha Printing Co., Ltd., Kyoto, Japan*

TP 100 **N-glycopeptides Analysis of Serum Alpha-1-antitrypsin in Liver Cirrhosis and Hepatocellular Carcinoma**; Mengmeng Wang[1, 2]; Jianhui Zhu[1]; Jing Liang[1, 3]; Tingting Chen[1]; Mingrui An[1]; Yifan Huang[4]; Yehia Mechref[4]; Chunfang Gao[2]; David M. Lubman[1]; *[1]Department of Surgery, University of Michigan Medical Center, Ann Arbor, MI; [2]Department of Laboratory Medicine, Eastern Hepatobiliary Surgery Hospital, Second Military Medical University, Shanghai, China; [3]School of Chemical Engineering and Technology, China University of Mining and Technology, Xuzhou, China; [4]Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX*

TP 101 **Improved Sensitivity for Protein Biomarker Quantitation in Mouse Plasma by Sample Pretreatment and Trap-Elute Micro-Flow LC-MS/MS**; Mingfei Zeng[1]; Huachuan Cao[1]; *[1]Eli Lilly and Company, Shanghai, China*

TP 102 **The Power of Quantitative Multiplexing- Combining TMT Discovery and Targeted Label Free Workflows for Biomarker Analysis**; Xiaoyue Jiang[1]; Katherine Herting[2]; Ramesh Ganapathy[2]; Sergei Snovida[2]; David Horn[3]; Vic Spicer[4]; Oleg Krokhin[4]; Rosa Viner[5]; Andreas F. Huhmer[5]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Rockford, IL; [3]Thermo Fisher Scientific, San Jose, CA; [4]University of Manitoba, Winnipeg, MB; [5]Thermo Fisher Scientific, San Jose, CA*

TP 103 **Quantitation of Stercobilin in the Fecal Material of Timothy Syndrome Mice as a Putative Biomarker for Autism**; Emily Sekera[1]; Troy D. Wood[1]; Heather L Rudolph[1]; Stephen Carro[1]; *[1]University at Buffalo, Buffalo, NY*

TP 104 **Oxyntomodulin Quantitation in Human Plasma: High Resolution Q-TOF Quantification Myths Debunked**; Megan Yajuan Wang[1]; Anita Lee[1]; Derek Chappell[1]; Omar Laterza[1]; Michael Lassman[1]; *[1]Merck Research Laboratories, Rahway, NJ*

TP 105 **Monitoring with Quantitation the Glycosylation of Multiple Glycoproteins for Diseases Biomarker Discovery**; Qiongyu Li[1]; Muchena J. Kailemia[1]; Frank Leon[2]; Emanual Maverakis[3]; Carlito B. Lebrilla[1]; *[1]Department of Chemistry, University of California, Davis, Davis, CA; [2]Biochemistry, Molecular, Cellular and Developmental Biology, University of California, Davis, Davis, CA; [3]Department of Dermotology, School of Medicine University of California, Davis, Sacramento, CA*

TP 106 **Site-Specific Glycopeptide Analysis of Human alpha-1-acid Glycoprotein (AGP)in Liver Cirrhosis and Hepatocellular Carcinoma of Different Etiologies**; Jing Liang[1, 2]; Jianhui Zhu[3]; Mingrui An[3]; Mengmeng Wang[3, 4]; Yifan Huang[5]; Yehia Mechref[6]; David M. Lubman[7]; *[1]University of Michigan Medical Center, Ann Arbor, Michigan; [2]School of Chemical Engineering and Technology, China University of Mining and Technology, Xuzhou, China; [3]University of Michigan Medical Center, Ann Arbor, MI; [4]Department of Laborary Medicine, Eastern Hepatobiliary Surgery Hospital, Second Military Medical University, Shanghai, China; [5]Department of Chemistry & Biochemistry, Texas Tech University, Lubbock, TX; [6]Department of Chemistry & Biochemistry, Texas Tech University, Lubbock, TX; [7]University of Michigan Medical Center, Ann Arbor, MI*

TP 107 **Oxysterol, Secosterols, and Cholesterol Intermediates Separation and Quantitation Using Triple Quadrupole Mass Spectrometry**; Evelyn H. Wang[1]; Jerry Byrne II[1]; Rachel Lieberman[1]; Sonia Bholanath Bhattacharya[2]; Richard W. Browne[2]; Christopher Gilles[1]; *[1]Shimadzu Scientific Instruments, Columbia, MD; [2]University of Buffalo, Buffalo, NY*

TP 108 **Orthogonal Proteomic Verification of Low Histone H4-K12,16Ac Levels in Homologous Recombination Deficient High-Grade Serous Ovarian Carcinomas**; Stefani Thomas[1]; Lijun Chen[1]; Yang Liu[1]; Naseruddin Höti[1]; Hui Zhang[1]; *[1]Johns Hopkins University, Baltimore, MD*

TP 109 **Capillary Electrophoresis-Mass Spectrometry**

Method Development for Biomarkers of Indoleamine 2,3-Dioxygenase; Yunan Wang[1]; Mei Han[1]; Jing Man Wong[1]; Dan A. Rock[1]; Brooke M. Rock[1]; *[1]Amgen, South San Francisco, CA*

TP 110 **Alpha-1 Antitrypsin Quantification using LC-MS/MS**; Qingguo Tian[1]; Bob Xiong[2]; Eric Lund[1]; Dawn Christianson[1]; Zhen Li[1]; *[1]Arrowhead Pharmaceuticals Inc., Madison, WI; [2]Covance, Durham, NC*

TP 111 **Mass Spectrometry based Proteomics Investigation of Induced Obstructive Sleep Apnea (OSA) in Rat Atria**; Devika Channaveerappa[1]; Jacob Lux[2]; Kelly L. Wormwood[2]; Meredith McLerie[2]; Brian Panama[2]; *[1]Clarkson University, Potsdam, NY; [2]Masonic Medical Research Laboratory, Utica, NY*

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TP 113 **Fast Pyrolysis of 13C- and 18O-Labelled Cellooligosaccharides: Probing the Mechanisms of Fast Pyrolysis of Carbohydrates by Using Tandem Mass Spectrometry**; Zaikuan Yu[1]; Priya Murria[1]; Mckay Easton[1]; Hilkka Kenttämaa[1]; *[1]Purdue University-Department of Chemistry, West Lafayette, IN*

TP 114 **Structural Characterization of Heparin and Heparan Sulfate using 193 nm Ultraviolet Photodisscoation**; Dustin Klein[1]; Jennifer S Brodbelt[2]; *[1]University of Texas at Austin, Austin, TX; [2]University of Texas at Austin, Austin, TX*

TP 115 **Resolution of Carbohydrate Isomers via Ion Mobility-Mass Spectrometry with Boronic Acid Shift Reagent**; Li Li[1]; Kristin M Mckenna[1]; Facundo M Fernandez[1]; *[1]School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA*

TP 116 **Evaluation of UV Detection as a Novel Method for Glycan Analysis**; Charles Nwosu[1]; Shuangqi Sally Liu[1]; May Zhu[1]; *[1]Takeda Pharmaceuticals International, Cambridge, MA*

TP 117 **Linkage and Anomeric Configuration Determination by Electrospray Ionization Tandem Mass Spectrometry**; Chia Yen Liew[1]; Shang-Ting Tsai[1]; Jien-Lian Chen[1]; Hsu Chen Hsu[1]; Shih-Pei Huang[1]; Yuan-Tseh Lee[1, 2]; Chi-Kung Ni[1, 3]; *[1]Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan; [2]Department of Chemistry, National Taiwan University., Taipei, Taiwan; [3]Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan*

TP 118 **Machine Learning Approach for *de novo* Glycan Sequencing**; Pengyu Hong[1]; Yang Tang[2]; Hui Sun[1]; Long Sha[1]; Catherine E Costello[2, 3]; Cheng Lin[3]; *[1]Brandeis University, Waltham, MA; [2]Boston University, Boston, MA; [3]Boston University School of Medicine, Boston, MA*

TP 119 **High Mannose Glycan Characterization and Quantitation by Free Radical Reagents**; Kimberly Fabijanczuk[1]; Jose Acosta[2]; Trang Do[2]; Jinshan Gao[2]; *[1], Montcalir, NJ - New Jersey; [2]Montclair State University, Montcalir, NJ*

TP 120 **Glycan Characterization and Quantitation by Free Radical Reagents**; Jinshan Gao[1]; Kaylee Gaspar[1]; Trang Do[1]; Nathaniel Adomako[1]; Kimberly Fabijanczuk[1]; Jose Acosta[1]; *[1]Montclair State University, Montcalir, NJ*

TP 121 **A Rapid LC-MS/MS-based Method for Carbohydrate Linkage Identification Using Multiple Reaction Monitoring (MRM)**; Ace G. Galermo[1]; Eshani Nandita[1]; Mariana Barboza[1, 2]; Matthew J. Amicucci[1, 3]; Thai-Thanh Vo[1]; Carlito B. Lebrilla[1]; *[1]Department of Chemistry, University of California, Davis, Davis, CA; [2]Department of Anatomy, Physiology, and Cell Biology, University of California, Davis, Davis, CA; [3]Agricultural and Environmental Chemistry Graduate Group, University of California, Davis, Davis, CA*

TP 122 **Novel 4-plex Isobaric Aldehyde Reactive N, N-Dimethyl Leucine Derivative Tags for Quantitative Glycomics Analysis**; Yu Feng[1]; Bingming Chen[1]; Qinying Yu[1]; Xuefei Zhong[1]; Lingjun Li[1, 2]; *[1]University of Wisconsin-Madison School of Pharmacy, Madison, WI; [2]University of Wisconsin - Madison Department of Chemistry, Madison, WI*

TP 123 **Comparative Study of in-ESI, Solution-Phase, and Gas-Phase Hydrogen/Deuterium Exchange for Conformational Analysis of Carbohydrate-Metal Adducts**; Tara Liyanage[1]; Matthew R Brantley[1]; Touradj Solouki[1]; Elyssia S Gallagher[1]; *[1]Baylor University, Waco, TX*

TP 124 **Sialyl Glycan Characterization by Free Radical Activated Glycan Structure Elucidation Reagent**; Kaylee Gaspar[1]; Trang Do[2]; Nathaniel Adomako[2]; Jinshan Gao[2]; *[1], Montclair, NJ; [2]Montclair State University, Montcalir, NJ*

TP 125 **Absolute Quantitation of Branching in Polysaccharides using Isotopically Differentiated Permethylation**; Eshani Nandita[1]; Ace G. Galermo[1]; Matthew J. Amicucci[2]; Mariana Barboza[3]; Carlito B. Lebrilla[1]; *[1]UC Davis Department of Chemistry, Davis, CA; [2]UC Davis Agricultural and Environmental Chemistry Graduate Group, Davis, CA; [3]UC Davis Department of Anatomy, Physiology, and Cell Biology, Davis, CA*

TP 126 **Differentiating Isomeric Disaccharides on the Different Types of Mass spectrometers**; Wei Mi[1]; Zhishang Hu[1]; Hongmei Li[1]; Changkun Li[2]; Jing Wang[1]; *[1]National Insititute of Metrology, Beijing, China; [2]Shimadzu Incorporated, Beijing, China*

TP 127 **New Applications and Technologies for INLIGHT™ N- and O-linked Glycans**; Samuel R. King[1]; Elizabeth S. Hecht[1]; Philip L. Loziuk[1]; Erin S. Baker[2]; David C. Muddiman[1]; *[1]North Carolina State University, Raleigh, NC; [2]Pacific Northwest National Laboratory, Richland, WA*

TP 128 **Formation of Doubly Alkali Metal-Cationized Monosialylated Fragments from Singly Alkali Metal-Cationized LSTb and GM1 during MALDI-MS/MS and ESI-MS/MS**; Krishani K. Rajanayake[1]; Kevin Markus[1]; Dragan Isailovic[1]; *[1]The University of Toledo, Toledo, OH*

TP 129 **Structural Elucidation of Fucosylated Chondroitin Sulfates from Sea Cucumber Using Electrospray Ionization Tandem Mass Spectrometry**; Isaac Agyekum[1]; Lauren Pepi[1]; Shiguo Chen[2]; Robert J Linhardt[3]; I Jonathan Amster[1]; *[1]University of Georgia,Chemistry Department, Athens, GA; [2]Zhejiang University, Department of Food Science and Nutrition, Hangzhou, China; [3]Rensselaer Polytechnic Institute, Troy, NY*

TP 130 **Sensitive Detection of Sialylated N-Glycans using Optimized HILIC LC-MS Separations**; Qi Wang[1]; Matthew A. Lauber[1]; *[1]Waters Corporation, Milford, MA*

TP 131 **Dextran Derivatization for Multiple Proton Adduct Ionization Using ESI-TOF Mass Spectrometry**; Jesus B. Tapia[1]; Hailey Hibbard[1]; Melissa M. Reynolds[1]; *[1]Colorado State University, Fort Collins, CO*

TP 132 **Optimization of Reverse Polarity Capillary Electrophoresis-Mass Spectrometry Separations for the Analysis of Sulfated Glycosaminoglycan Oligosaccharide Mixtures**; Morgan Stickney[1]; Patience Sanderson[1]; Franklin E Leach III[1]; James Xia[2]; Yanlei Yu[3]; Fuming Zhang[3]; Robert J Linhardt[3]; I. Jonathan Amster[1]; *[1]University of Georgia, Athens, GA; [2]CMP Scientific, Corp., Brooklyn, N.Y.; [3]Rensselaer Polytechnic Institute, Troy, NY*

TP 133 **Negative Electron Transfer Dissociation Sequencing of Increasingly Sulfated Glycosaminoglycan Oligosaccharides in an Orbitrap Mass Spectrometer**; Franklin E. Leach III[1]; Nicholas M. Riley[2]; Matthew J. P. Rush[2]; Michael S. Westphall[2]; Joshua J. Coon[2]; I. Jonathan Amster[1]; *[1]University of Georgia, Athens, GA; [2]University of Wisconsin, Madison, WI*

TP 134 **Rapid and Sensitive MALDI MS Analysis of**

Oligosaccharides by using 2-hydrazinopyrimidine as a Derivative Reagent and Co-Matrix; Kuan Jiang[1]; Arya Aloor[2]; Jiangyao Qu[3]; Cong Xiao[3]; Zhigang Wu[3]; Cheng Ma[3]; Peng Wang[3]; *[1]Nankai University, Tianjin; [2]Georgia State University, Atlanta, GA; [3]Georgia State University, Atlanta, GA*

TP 135 **From Computation to Mass Spectrometry: Relative Free Energy Differences amongst Anomeric Pairs of Carbohydrate Derivatives**; Gabe Nagy[1]; Alison E. Vickman[1]; Nicola L. B. Pohl[1]; *[1]Indiana University Bloomington, Bloomington, IN*

TP 136 **Does Low Energy CID Always Occur on the Reducing End of Carbohydrate?**; Shang-Ting Tsai[1]; Chia Yen Liew[2]; Shih-Pei Huang[2]; Yuan-Tseh Lee[2, 3]; Chi-Kung Ni[2, 4]; *[1]Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan; [2]Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan; [3]Department of Chemistry, National Taiwan University., Taipei, Taiwan; [4]Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan*

TP 137 **Incorporating Mass Spectrometry into Biologic QC Control Environments for O- Glycan Analysis**; Mark Hilliard[1]; Ciara McManus[1]; William Alley[2]; Ying Qing Yu[2]; Pauline Rudd[1]; *[1]NIBRT, Dublin, Ireland; [2]Waters Corporation, Milford, MA*

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TP 139 **Analysis of Protein-Protein Interactions by Data-Dependent Acquisition without Dynamic Exclusion**; Shen Zhang[1]; Brett Larsen[2]; Anne-Claude Gingras[2]; *[1]Lunenfeld-Tanenbaum Research Institute, Toronto, Ontario; [2]Lunenfeld-Tanenbaum Research Institute, Toronto, ON*

TP 140 **Developing and Executing Advanced Data-Dependent Acquisition Strategies for Proteomics in MaxQuant-RealTime**; Christoph Wichmann[1]; Florian Meier[1]; Matthias Mann[1]; Juergen Cox[1]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany*

TP 141 **Evaluation of a Peptide Selection Algorithm for Trapped Ion Mobility with Parallel Accumulation Serial Fragmentation (TIMS-PASEF) on a Q-TOF Instrument**; Markus Lubeck[1]; Stephanie Kaspar-Schoenefeld[1]; Niels Goedecke[1]; Oliver Raether[1]; Scarlet Beck[2]; Heiner Koch[2]; Florian Meier[2]; Juergen Cox[2]; Matthias Mann[2]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Max Planck Institute of Biochemistry, Martinsried, Germany*

TP 142 **Laser-Induced Dissociation Combined with Data Independent Acquisition (DIA-LID) : A Proof of Concept Study Covering Human Kinome Expression**; Lény Garcia[1]; Marion Girod[1]; Magali Rompais[2]; Philippe Dugourd[3]; Christine Carapito[2]; Jérôme Lemoine[1]; *[1]Institut des Sciences Analytiques, Université de Lyon, Université Lyon 1, Ens de Lyon, CNRS, Lyon, France; [2]Laboratoire de Spectrométrie de Masse BioOrganique, University of Strasbourg, Strasbourg, France; [3]Institut Lumière Matière, Université de Lyon, Université Lyon 1, CNRS, Lyon, France*

TP 143 **Deciphering Heterochromatin Proteome with Next Generation Proteomics**; Tania Auchynnikava[1]; Lauri Peil[2]; Piotr Grabowski[3]; Alison Pidoux[4]; Ryan Ard[4]; Robin Allshire[4]; Juri Rappsilber[3, 4]; *[1]University of Edinburgh, Edinburgh; [2]University of Tartu, Tartu, Estonia; [3]Technical University Berlin, Berlin, Germany; [4]University of Edinburgh, Edinburgh, UK*

TP 144 **Maximizing Proteome Coverage through Judicious Selection of Quadrupole Ion Trap Settings and Improved On-Line Orbitrap Peak Annotation**; Graeme McAlister[1]; Christian Thoeing[2]; Romain Huguet[1]; Alex Hebert[3]; Philip M Remes[1]; Andreas Kuehn[2]; Vlad Zabrouskov[1]; Joshua J. Coon[3]; Mike Senko[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Bremen, Germany; [3]University of Wisconsin Madison, Madison, WI*

TP 145 **The Advantages of Using an MRMHR Acquisition for Increased Sensitivity for Targeted Analysis Using a QTOF Instrument**; Paul C. Winkler[1]; K.C. Hyland[2]; Christopher Borton[2]; *[1]SCIEX, Framingham, MA; [2]SCIEX, Redwood City, CA*

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TP 147 **Quantitation of Triptorelin in Rat Plasma Using Triple Quadrupole Mass Spectrometry**; Ting Liu[1]; Lin Zhu[2]; Wenhai Jin[3]; Xiongwei Yang[2]; Jingsheng Zhang[2]; Jifeng Deng[2]; *[1]SCIEX, Shanghai, China; [2]SCIEX, Guangzhou; [3]SCIEX, Beijing, China*

TP 148 **Applying High Energy In-Source Fragmentation to Quantify Complex Cationic Lipids in Pharmacokinetic Studies using LC/MS** ; Nanyan Rena Zhang[1]; Sean Yu[2]; William Bart Emary[1]; *[1]Merck, West Point, PA; [2]RMI Laboratories, North Wales, PA*

TP 149 **Unique Challenges for LC-MS/MS Analysis of the Phosphorylated Metabolites of a Nucleoside Analog in Human Peripheral Blood Mononuclear Cells**; Li Sun[1]; Cynthia Chavez-Eng[1]; Sheila Breidinger[1]; Kerry Fillgrove[1]; Bing Lu[1]; Eric Woolf[1]; *[1]Merck Research Labs, Merck & Co,, West Point, PA*

TP 150 **Evaluation of Noviplex Card for Plasma Concentration Determination**; Lingling Xue[1]; Yang Xu[1]; James Schiller[1]; guangping Bi[1]; Michelle Groff[1]; Jane Harrelson[1]; *[1]Merck & Co., Inc., West Point, PA*

TP 151 **High Resolution Accurate Mass Assays for the Quantitation of Abiraterone in Human Plasma**; Atul Bhatnagar[1]; Matthew J McKay[1, 2]; Megan Crumbaker[3]; Howard Gurney[4]; Mark P Molloy[1, 2]; *[1]Chemistry & Biomolecular Sciences, Macquarie University, North Ryde, Sydney, Australia; [2]Australian Proteome Analysis Facility, Macquarie University, North Ryde, Sydney, Australia; [3]Crown Princess Mary Cancer Centre, Westmead Hospital, Westmead, Australia; [4]Macquarie University Hospital, North Ryde, Sydney, Australia*

TP 152 **Experimental Investigation of the Factors Affecting the Sensitivity of HPLC/MS Coupled with Ion-Molecule Reactions**; Ravikiran Yerabolu[1]; Raghavendhar R Kotha[1]; John Kong[1]; Zaikuan Yu[1]; Rashmi Kumar[1]; Chungang Gu[2]; Hilkka Kenttamaa[1]; *[1]Purdue University, West Lafayette, IN; [2]AstraZeneca R&D, Waltham, MA*

TP 153 **Development of High-Performance Micro-flow LC-MS/MS Methodology and Application to a High-Throughput Screening Workflow**; Brendon Kapinos[1]; John Janiszewski[1]; Hui Zhang[1]; Jianhua Liu[1]; Brian Holder[1]; Wayne Lootsma[2]; Steve Ainley[2]; Amanda Berg[3]; Erik Hansen[3]; *[1]Pfizer Inc., Groton, CT; [2]Sound Analytics, Niantic, CT; [3]New Objective, Woburn, MA*

TP 154 **Understanding Metabolism of an Achiral Drug to Chiral Metabolites in Biological Matrices using SFC-QQQ Technology**; Siji Joseph[1]; Syed Salman Lateef[2]; *[1]Agilent technologies, Bangalore, Karnataka; [2]Agilent Technologies India, Bangalore, India*

TP 155 **Online Solid Phase Extraction LC/MS/MS Analysis**

of 3-Methoxytyramine, Normetanephrine and Metanephrine in Urine: A Unique Approach; Xiaoning Lu[1]; David S. Bell[1]; *[1]MilliporeSigma, Bellefonte, PA*

TP 156 **Comparison of Combining Quantitative with Qualitative Met ID Analysis in the QTrap 6500 and Triple TOF 5600 Mass Spectrometer**; Minli Zhang[1]; Keith J. Goodman[2]; Diane L. Nabb[1]; Heather Peterson[1]; John M. Hevko[2]; *[1]DuPont, Newark, DE; [2]Sciex, Framingham, MA*

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TP 158 **High-Resolution Mass Spectrometry for Efficient Identification of the Transformation Products of Aromatic Emerging Contaminants in Chlorinated Water**; Wen-Ling Chen[1]; Jiun-Yi Cheng[1]; *[1]Department of Environmental Science and Engineering, College of Engineering, Tunghai University, Taichung, Taiwan*

TP 159 **Application of Paper Spray Differential Ion Mobility Mass Spectrometry for Pesticide Products Screening**; Khang To; *University of North Carolina, Chapel Hill, NC*

TP 160 **MS-MS Studies of the Partitioning and Recovery of Pesticides Interacting with Soils**; Heather Gamble[1]; Miles Snow[2]; Donald S Gamble[3]; *[1]Perkin Elmer Health Sciences, Bolton, ON; [2]PerkinElmer LAS Canada Inc, Woodbridge, ON; [3]Department of Chemistry, St. Mary's University, Halifax, NS*

TP 161 **An Innovative Liquid-El Interface Coupled to UHPLC for Analysis of Xenobiotics, Exemplified with Organochlorine Pesticides in Soil Matrix**; Veronica Termopoli[1]; Giorgio Famiglini[1]; Pierangela Palma[1]; Maurizio Piergiovanni[1]; Achille Cappiello[1]; Simon Perry[2]; Mansoor Saeed[2]; *[1]University of Urbino, Urbino, Italy; [2]SYNGENTA, Bracknell, UK*

TP 162 **Fast Scanning and Sensitivity for Real-Time Confirmation of Structural Isoforms using a High Performance Triple Quadrupole Mass Spectrometer**; Alan Atkins; *Thermo Fisher Scientific-, Hemel Hempstead, UK*

TP 163 **One-Step Extraction and Concentration for Identifying Pharmaceuticals and Personal Care Products in Water, Biosolids and Solids** ; Matt Falkenstein[1]; Philip Bassignani[1]; *[1]Fluid Management Systems, Watertown, MA*

TP 164 **High-Speed Formaldehyde Analysis for the Process-Line and Laboratory: SIFT-MS**; Murray J Mcewan[1]; Mark Perkins[2]; Daniel B Milligan[3]; Barry J Prince[3]; Vaughan S Langford[3]; *[1]University of Canterbury, Christchurch, Canterbury; [2]Anatune Limited, Cambridge, UK; [3]Syft Technologies Ltd, Christchurch, New Zealand*

TP 165 **Improved Quantitation of Fragile Carbamate, Organophosphate, and Other Pesticides by Automatic MS/MS Method Generation**; Eric Huang[1]; Bennett Kalafut[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

TP 166 **A Rapid LCMS Method for Evaluating PPCPs Contamiants Found in Drinking Water**; Katie Pryor[1]; Rachel A Liberman[1]; Christopher T Gilles[1]; *[1]Shimadzu Scientific Instr., Columbia, MD*

TP 167 **Analysis of Persistent Organic Pollutants in Atmospheric Aerosol using a Novel Ultrasound Assited Extraction Micro-Scale Cell and GCMS-QQQ System**; Eleazar Rojas Santiago[1]; Gelasio Perez Valverde[1]; Erik Beristain Montiel[2]; Eliana Arias Loaiza[2]; Omar Amador Muñoz[2]; *[1]Agilent Technologies Mexico, Mexico City, Mexico; [2]centro de Ciencias de la Atmosfera UNAM, Mexico City, Mexico*

TP 168 **Scanning-SWATH for Pesticide Analysis and Quantitation**; Nic Bloomfield[1]; J.C. Yves Leblanc[1]; Gordana Ivosev[1]; Ian Tremble[1]; Jamie Sherman[1]; Andre Schreiber[1]; *[1]SCIEX, Concord, ON*

TP 169 **Smart Target Method Development Based on Suspect Screening and HRMS for Detection of Antidiabetic Compounds in Wastewater and Surface Water**; Damia Barcelo[1, 2]; Bozo Zonja[1]; Juan Carlos Guillen[1]; Miren López de Alda[1]; *[1]IDAEA-CSIC, Barcelona, Spain; [2]ICRA, Girona, Spain*

TP 170 **Analysis of Genotoxic Impurities Like Ethane Sulfonic Acid Esters in Pharmaceutical Substance by GCMS/MS**; Prashant Hase[1]; Ankush Bhone[1]; Durvesh sawant[1]; Dheeraj Handique[1]; Sanket Chiplunkar[1]; Nitish Suryawanshi[1]; Ajit Datar[1]; Jitendra Kelkar[1]; Pratap Rasam[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

TP 171 **A New, Fast, Simple, and Ultra-Sensitive Determination of Semi-Volatile Organic Compounds in Water Samples by GC-MS/MS Triple Quadrupole System**; Diego Martín-Ortiz[1]; Javier López[1]; Miguel Ángel Pérez[1]; Cory Lytle[2]; Louis Maljers[2]; *[1]Bruker Espanola S.A., Madrid, Spain; [2]Bruker Daltonics Inc., Billerica, MA*

TP 172 **Determination of Pesticide Residues for Quality Control of Tobacco Products by LC/MS/MS**; Prasanth Joseph[1]; Samir Vyas[2]; *[1]Agilent Technologies, Bangalore, India; [2]Agilent Technologies India, Manesar, India*

TP 173 **New Platforms for Environmental (Bio)monitoring**; Geuncheol Gil[1]; Pan Mao[1]; Daojing Wang[1]; *[1]Newomics Inc., Emeryville, CA*

TP 174 **Ultra-trace Analytical Method for the Quantification of Pyrethroid and Organophosphate Insecticides in Surface Water using Passive Sampler Membranes and GC-APCI-MS/MS**; Birgit Beck[1]; Christoph Moschet[2]; Juliane Hollender[1]; Heinz Singer[1]; *[1]Eawag, Duebendorf, CH; [2]Cantonal Laboratory for the Environment, Schaffhausen, Switzerland*

TP 175 **Isolation and Identification of Priority Contaminants of Emerging Concern and Their Transformation Products: Use of UPLC QTof MS/MS**; Hlengilizwe Nyoni[1]; Bhekie B. Mamba[1]; Titus A.M. Msagati[1]; *[1]University of South Africa, College of Science Engineering and Technology, Nanotechnology and Water Sustainability, UNISA Science Campus, Florida, Johannesburg, South Africa*

TP 176 **Measuring Emerging Contaminant Degradation in Anaerobic Digestion or Composting Systems by Liquid-Liquid Extraction and LC-QQQ-MS**; Lisa Wolfe[1]; Vicki Larson[2]; Corey D. Broeckling[3]; Jessica E. Prenni[3]; Susan DeLong[2]; *[1]Proteomics and Metabolomics Facility; Colorado State University, Fort Collins, CO; [2]Department of Civil and Environmental Engineering, Colorado State University, Fort Collins, CO; [3]Proteomics and Metabolomics Facility; Colorado State University, Fort Collins, CO*

TP 177 **Liquid Chromatography-High Resolution Mass Spectrometry as a Powerful Tool of High Volume Screening of Emerging Contaminants in Wastewater**; Alice Tendai Hungwe[1]; Vimbai Mhuka[1]; Simiso Dube-Nindi[1]; Mathew Nindi[2]; *[1]Department of Chemistry, College of Science, Engineering and Technology, the Science Campus, University of South Africa,, Florida Park, Roodepoort, Johannesburg, 1709, South Africa, South Africa; [2]University of South Africa, Pretoria, Gauteng*

TP 178 **Automated Online SPE/Tandem-MS Analysis of Trace Organic Contaminants in Drinking Water**; Patrick M Batoon[1]; Theresa Sosienski[2]; Dan-Hui Dorothy Yang[2]; Tarun Anumol[3]; Craig Marvin[3]; Patrick Jeanville[2]; *[1]Agilent Technologies Inc., Santa Clara, CA; [2]Agilent Technologies, Inc., Santa Clara, CA; [3]Agilent Technologies, Inc., Wilmington, DE*

TP 179 **Quantitation of Pharmaceutical and Personal Care**

Products in Water using a Laminar Flow Tandem Mass Spectrometer; Jamie Foss[1]; Sharanya Reddy[1]; *[1]PerkinElmer Inc, Shelton, CT*

TP 180 **Photochemical Degradation of Phenols in Water using Flavin-Based Photosensitizers**; Quan Wang[1]; Brock Allen[2]; Xiaobo Yin[1]; Hui Ding[3]; Liang Xue[4]; *[1]Central South University, Changsha, China; [2]University of the Pacific, Stockton, CA; [3]UCLA, Los Angeles, California; [4]University of the Pacific, Stockton, CA*

TP 181 **Evaluation of Matrix Interferences on a Multiresidue Pesticide Analysis in Different Commodities using LC-QQQ**; Victor Manuel Mondragon Olguin; *Agilent Technologies Mexico, Mexico City, Mexico*

TP 182 **Pharmaceuticals and Personal Care Products (PPCPs) in Surface Water**; Jerry Byrne II[1]; Evelyn Wang[1]; Christopher Gilles[1]; *[1]Shimadzu Scientific Instruments, Columbia, MD*

TP 183 **Effects of Temperature and Hydrodynamic Conditions on Pocis Sampling rates for Constant Concentration Exposures**; Valerie Toteu Djomte[1]; Kevin Chambliss[1]; *[1]Baylor University, Waco, TX*

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TP 184 **Sensitive and Fast Measurement of Aminoglycoside Antibiotics in Milk, Meat or Eggs by HILIC-MS/MS and Identification using MRM Spectrum Mode**; Mikael LEVI[1]; Hisashi Kato[2]; David Baker[3]; Ichiro Hirano[1]; *[1]Shimadzu Corp., MS BU, Kyoto, Japan; [2]BIOTAGE Japan, Tokyo, Japan; [3]Shimadzu MSBU Overseas, Manchester, UK*

TP 185 **Multi-residue Analysis of 18 Regulated Mycotoxins by LC-MS/MS in Food Samples**; David Baker[1]; Chris Titman[1]; Jonathan Horner[2]; Neil Loftus[1]; Bart Jansen[3]; *[1]Shimadzu, Manchester, UK; [2]Scientific Analysis Laboratories, Cambridge, UK; [3]Shimadzu Benelux, Hertogenbosch, Netherlands*

TP 186 **Analyzing Spent Grains as a Sustainable Source of Feed**; Liesl Krone[1]; BJ Bench[2]; Manju Bala[3]; Andre Schreiber[4]; Jennifer Krone[5]; Oscar Cabrices[6]; *[1]Granbury High School, Granbury, TX; [2]Food Safety and Research Laboratory Tyson Foods, Springdale, AR; [3]CPS, PLLC, Brentwood, TN; [4]SCIEX, Darmstadt, Germany; [5]SCIEX, Redwood City, CA; [6]GERSTEL, Inc, Linthicum, MD*

TP 187 **Determination of Mancozeb in Flammulina Velutipes by UPLC-MS/MS**; Guihong Cheng[1]; Xiang Li[2]; Feng Qin[3]; Cai Chengyuan[2]; Lizhong Yang[2]; Zhou Xiangdong[2]; *[1]Sichuan FDA, Chengdu, China; [2]PerkinElmer Management (Shanghai) Co, Shanghai, China; [3]PerkinElmer LAS Canada Inc, Woodbridge*

TP 188 **Simultaneous Determination of Pesticides Residues and Illegal Additives in Wine by Ultra-Performance Liquid Chromatography Tandem Mass Spectrometry**; Minli Zhu[1]; Weifeng Zhang[1]; Lina Tang[2]; Lizhong Yang[3]; Xaingdong Zhou[3]; Chengyuan Cai[3]; Feng Qin[4]; Xiang Li[3]; Yongming Xie[3]; *[1]Guangzhou Agricultural Products Quantity and Safety Supervisory Institute, Guangzhou, China; [2]Xiamen Entry-Exit Inspection and Quarantine Bureau, Xiamen, China; [3]PerkinElmer Management (Shanghai) Co, Shanghai, China; [4]PerkinElmer LAS Canada Inc, Woodbridge, ON*

TP 189 **Determination of Polycyclic Aromatic Hydrocarbonsin Seafood and Edible Oil by Ultra-Performance Liquid Chromatography Tandem Mass Spectrometry**; Min Wu[1]; Jin Zhang[1]; Lizhong Yang[2]; Chengyuan Cai[2]; Xiangdong Zhou[2]; Zhuo Man[2]; Feng Qin[3]; Xiang Li[2]; Yongming Xie[2]; *[1]Xiamen Entry-Exit Inspection and Quarantine Bureau, Xiamen, China; [2]PerkinElmer Management (Shanghai) Co., Ltd. Shanghai, China, Shanghai, China; [3]PerkinElmer LAS Canada Inc, Toronto, ON*

TP 190 **Analysis of Pesticide Residues in Cannabis Regulated by Oregon State using LC-MS/MS**; Sharanya Reddy[1]; Ben Armstrong[2]; Steve Stadlmann[2]; Toby Astill[3]; *[1]PerkinElmer, Shelton, CT; [2]Juniper Labs, Bend, Oregon; [3]PerkinElmer Inc., San Jose, CA*

TP 191 **Pesticide Analysis in Hops and Cannabis by GC-MS-MS**; Jeff Dahl[1]; Riki KItano[2]; Julie Kowalski[3]; *[1]Shimadzu, Columbia, MD; [2]Shimadzu Scientific Instr., Columbia, MD; [3]Restek Corporation, Bellefonte, PA*

TP 192 **Solid Phase Extraction Based Pass-Through Clean-Up for Multi-Class Analysis of Veterinary Drugs in Baby Food Containing Milk Powder using LC-MS/MS**; Ujwal Patil[1]; Sarah Ruiz[1]; Cheryl Stephenson[1]; John Reuther[1]; *[1]Eurofins CAL, New Orleans, LA*

TP 193 **Identification of Sweeteners in E-liquids by Electrospray Ionization Mass Spectrometry**; Katherine D. Murdoch[1]; James E. Keating[1]; Nicholas J. Wallbillich[1]; Gary L. Glish[1]; *[1]University of North Carolina at Chapel Hill, Department of Chemistry, Chapel Hill, NC*

TP 194 **Applying 'MRM Spectrum Mode' and Library Searching for Enhanced Reporting Confidence in Routine Pesticide Residue Analysis**; David Baker[1]; Chris Titman[1]; Jonathan Horner[2]; Neil Loftus[1]; *[1]Shimadzu, Manchester, UK; [2]Scientific Analysis Laboratories, Cambridge, UK*

TP 195 **Analysis of Toxic Elements in Processed Milk Products using Inductive Coupled Plasma Mass Spectrometry (ICPMS)**; Mangesh Pawar[1]; Sampada Khopkar[1]; Ankush Bhone[1]; Amol Shinde[1]; Ajit Datar[1]; Jitendra Kelkar[1]; Pratap Rasam[1]; *[1]Shimadzu Analytical India Pvt. Ltd., Mumbai, Maharashtra*

TP 196 **The Analysis of Polar Ionic Pesticides by Ion-Exchange Chromatography Tandem Mass Spectrometry: The Possible Solution to a Longstanding Problematic Analysis?**; Jonathan Beck[1]; Stuart Adams[2]; Michael Dickinson[2]; Ed George[3]; Jonathan Guest[2]; Richard Fussell[4]; *[1]ThermoFisher Scientific, San Jose, CA; [2]FERA, Sand Hutton, UK; [3]ThermoFisher, San Jose, CA; [4]Thermo Fisher Scientific, Bremen, Germany*

TP 197 **Analysis of Mycotoxins in Food Matrices using HPLC/MS/MS**; Theresa Sosienski[1]; Dan-Hui Dorothy Yang[1]; Joan Stevens[2]; Christian Hegmanns[3]; Patrick Jeanville[1]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]Agilent Technologies, Inc., Wilmington, DE; [3]Agilent Technologies Sales & Services GmbH & Co. KG, Waldbronn, Germany*

TP 198 **Multi-residual Quantitative Analytical Method for Antibiotics in Sea Food by LC/MS/MS**; Anant Lohar[1]; Shailendra Rane[1]; Rashi Kochhar[1]; Ashutosh Shelar[1]; Shailesh Damale[1]; Purushottam Sutar[1]; Deepti Bhandarkar[1]; Ajit Datar[1]; Pratap Rasam[1]; Jitendra Kelkar[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

TP 199 **Target Screening of Multi-Class Antibiotic Residues in Raw Milk using UHPLC Eletrospray Ionization Orbitrap Mass Spectrometry**; Daniel Leung[1]; Jian Wang[1]; Willis Chow[1]; James Chang[2]; *[1]Canadian Food Inspection Agency, Calgary, Alberta; [2]Thermo Fisher Scientific, San Jose, CA*

TP 200 **I Knew You Were Trouble: Expanding LC Methods to Include Difficult GC Compounds using a Novel Ionization Technique**; Susan Leonard[1]; Kari Organtini[1]; Gareth Cleland[1]; Gordon Fujimoto[2]; Kenneth Rosnack[1]; Ramesh P Rao[3]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Beverly, MA; [3]Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK*

TP 201 **Sensitive and Specific Allergen Screening Analysis Using LC-MS/MS**; Paul C. Winkler[1]; Hua-Fen Liu[2]; Christopher Borton[2]; Leesun New[2]; *[1]Sciex, Framingham, MA; [2]SCIEX, Redwood City, CA*

TP 202 **Simultaneous Analysis of Major Allergens in Food Matrices by High Sensitive Mass Spectrometer**; Tairo Ogura; *Shimadzu Scientific Instruments, Inc., Columbia, MD*

TP 203 **Simultaneous Determination of 16 Mycotoxins**

in Cereals using Stable Isotope Labeled Internal Standards and UHPLC-MS/MS; Qilei Guo[1]; Jian zhong Li[1]; Tao Bo[1]; *[1]Agilent Technologies, Beijing, China*

TP 204 **Development of a Multi-Residue Confirmatory Method for Determination of Sedatives by HPLC-MS/MS**; Pavel Metalnikov [1]; Ilya Batov[1]; Renat Selimov[1]; Alexander Komarov[1]; *[1]VGNKI, Moscow , Moscow*

TP 205 **On-Line Liquid-Liquid-Gas Chromatogrpahy-FID/QQQ MS for Mineral Oil Saturated and Aromatic Hydrocarbons Determination in Vegetable Oil**; Mariosimone Zoccali[1]; Paola Dugo[1, 2, 3]; Luigi Mondello[1, 2, 3]; *[1]Chromaleont s.r.l., Messina, Italy; [2]Dipartimento di Scienze Chimiche, Biologiche, Farmaceutiche ed Ambientali, University of Messina, Messina, Italy; [3]Unit of Food Science and Nutrition, Department of Medicine, University Campus Bio-Medico of Rome, Roma, Italy*

TP 206 **An Automated Technique for Multiresidue Analysis of Pesticides in Agricultural Samples**; Rudolf Addink[1]; Hamid R Shirkhan[1]; *[1]Toxic Report, Watertown, MA*

TP 207 **Multi-residue Veterinary Drug Analysis of >200 Compounds using MRM Spectrum Mode by LC-MS/MS**; David Baker[1]; Laetitia Fages[2]; Eric Capodanno[2]; Neil Loftus[1]; Simon Ashton[1]; *[1]Shimadzu, Manchester, UK; [2]Phytocontrol, Nimes, France*

TP 208 **Multi-Residue Pesticide Analysis in Food Matrices using HPLC/MS/MS**; Theresa Sosienski[1]; Dan-Hui Dorothy Yang[1]; Joan Stevens[2]; Patrick Jeanville[1]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]Agilent Technologies, Inc., Wilmington, DE*

TP 209 **Matrix-effect Free Quantitative Analysis using Nanoflow Liquid Chromatography High Resolution Mass Spectrometry**; David Moreno-González[1]; Jaime Alcantara-Durán[1]; Antonio Molina-Díaz[1]; Juan F Garcia-Reyes [1]; *[1]university of Jaen, Jaen , Andalucia*

TP 210 **Solid Phase Extraction and SFC-MS/MS Method for Analysis of Aflatoxins M1, M2, B1, B2, G1 and G2 in Milk Powders**; Jun Xiang Lee[1]; Yin Ling Chew[1]; Zhaoqi Zhan[1]; Jie Xing[1]; *[1]Shimadzu (Asia Pacific) Pte Ltd, Singapore*

TP 211 **Development of Sensitive and Selective Methods for Identification of Marine Toxins by Liquid Chromatography Tandem Mass Spectrometry**; Manami Kobayashi[1]; Junichi Masuda[1]; Yoshihiro Hayakawa[2]; *[1]Shimadzu Corporation, Hadano-city, Japan; [2]Shimadzu Corporation, Kyoto-city, Japan*

TP 212 **Determination of Chemical Contaminants in Indian Prawns by Fast GC-MS/MS using Modified QuEChERS as an Extraction Method**; Durvesh Sawant[1]; Prashant Hase[1]; Jitendra Kelkar[1]; Ankush Bhone[1]; Sanket Chiplunkar[1]; Dheeraj Handique[1]; Nitish Suryawanshi[1]; Ajit Datar[1]; Pratap Rasam[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

TP 213 **A Streamlined Multi-Residue Method for Quantitation and Confirmation of Selected Veterinary Drug Residues in Milk by High-Resolution Mass Spectrometry**; Kithsiri B Herath[1]; Hernando Escobar[1]; Lauren A. Girard[1]; Sherri B. Turnipseed[2]; Philip J. Kijak[1]; Hiranthi Jayasuriya[1]; *[1]Center for Veterinary Medicine/FDA, Laurel, MD; [2]U.S. Food and Drug Administration, Denver, CO*

TP 214 **DART-FTMS Detection of Melamine-Lactose Adducts and Condensation Products in Experimentally Adulterated Milk Powders**; Peter Scholl [1]; Luke K Ackerman[1]; Joseph H LaPointe[2]; Zhuohong Xie[3]; Jeffrey C Moore[3]; *[1]US FDA, College Park, MD; [2]IonSense Inc., Saugus, MA; [3]U.S. Pharmacopeia, Rockville, MD*

TP 215 **Development of Compounds Identification by Using Various Chromatography and Multiple Mass Spectrometry in Food Adulteration**; Chun-Ye Sun[1]; Shao-Zhen Wang[1]; Heng-Tao Dong[1]; *[1]Agilent Technology, Inc., Shanghai, China*

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TP 217 **Multivariate Data Analysis in the Interpretation of GC-MS fire Debris Results**; Marco Pazzi[1]; Laura Pacifici[1]; Eugenio Alladio[1, 2]; Fabrizio Malaspina[3]; Marco Vincenti[1, 2]; *[1]Dipartimento di Chimica, Università degli Studi di Torino, Torino, Italy; [2]Centro Regionale Antidoping e di Tossicologia "A. Bertinaria", Regione Gonzole 10/1, 10043 Orbassano (Torino), Italy; [3]Corpo Nazionale Vigili del Fuoco - Comando di Torino, Unità di Intervento Nucleare Biologico Chimico Radiologico, Torino, Italy*

TP 218 **Quantitation of THC and Metabolites in Whole Blood By LC-MS/MS For Per Se Law Testing**; Diana Tran[1, 2]; Xiang He[2]; Tracy Blethen[2]; Kevin Kopp[3]; Matt Kopp[3]; Alexandre Wang[2]; Hua-Fen Liu[2]; *[1], Redwood City, CA; [2]SCIEX, Redwood City, CA; [3]UTAK Laboratories Inc, Valencia, CA*

TP 219 **Multi-targeted Screening Procedures to Detect Prohibited Substances by LC-MS-based Techniques in Doping Control: Evaluation of Different Extraction Protocols**; Fabio Comunità[1]; Xavier de la Torre[1]; Monica Mazzarino[1]; Francesco Botrè[1, 2]; *[1]Antidoping laboratory of Rome, Rome, Italy; [2]Università Degli Studi di Roma "Sapienza", Rome, Italy*

TP 220 **Doping Control Analysis of Two Major JWH-250 Urinary Metabolites, JWH-250 4-OH-pentyl and JWH-250 5-OH-pentyl, in Equine urine by LC-MS/MS**; Youwen You[1, 2]; Rachel M. Proctor[1, 2]; Eric D. Vasilko[1, 2]; Mary A. Robinson[1, 2]; *[1]University of Pennsylvania, Kennett Square, PA; [2]PA Equine Toxicology & Research Laboratory, West Chester, PA*

TP 221 **Drug Analysis in Urine by Thermal Desorption and Pyrolysis Combined with DART-MS (TDP/DART-MS)**; Hiroko Abe[1]; Chikako Takei[2]; Yasuo Shida[2]; Motoshi Sakakura[3]; Teruhisa Shiota[3]; Kayako Suga[4]; Daisuke Yajima[1]; Hirotaro Iwase[1, 5]; *[1]University of Chiba, Chiba, Japan; [2]BioChromato, Inc., Fujisawa, Japan; [3]AMR Inc., Meguro-ku, Japan; [4]SCIEX, Shinagawa, Japan; [5]University of Tokyo, Bunkyo, Japan*

TP 222 **Strategies for Multiple-Target Screening using LC-MS/MS with Merged Spectrum Database for Forensic Toxicology**; Toshikazu Minohata[1]; Yutaro Yamamura[1]; *[1]Shimadzu Corporation, Kyoto, Japan*

TP 223 **A Novel Liquid Chromatography Tandem Mass Spectrometry Method Detection of Deinagkistrodon acutusvenom *in vivo***; Hangqi Li[1]; Jia Lin[1]; Chao Zhang[2]; Peibin Qin[2]; Huaidong Yu[2]; *[1]Institute of Forensic Science of Fujian Public Security Department, Fuzhou, China; [2]SCIEX Asia Pacific Application Support Center, Beijing, China*

TP 224 **Rapid Analysis of Protein Toxins using Hot Acid Digestion and MALDI-TOF with Post-Source Decay**; Dapeng Chen[1]; Wayne A. Bryden[2]; Catherine Fenselau[1]; *[1]Department of Chemistry and Biochemistry, University of Maryland, College Park, MD; [2]Zeteo Tech LLC, Ellicott City, MD*

TP 225 **The Utility and Legality of Using Portable, Ambient Sampling Mass Spectrometers in Traffic Stops**; Alessandra M. Bruno[1]; Scott Cleary[1]; Michael C. Gizzi[2]; Christopher C. Mulligan[1]; *[1]Department of Chemistry, Illinois State University, Normal, IL; [2]Department of Criminal Justice Sciences, Illinois State University, Normal, IL*

TP 226 **The Advantages of Direct Analysis of Morphine and its Metabolites with Related Compounds in Urine by LC-MS/MS**; Justin Steimling[1]; Frances Carroll[1]; Susan Steinike[1]; *[1]Restek Corporation, Bellefonte, PA*

TP 227 **A New Algorithm for Identifying Emerging Designer**

Drugs – A Case Study using Fentanyl; Arun S Moorthy[1]; William E Wallace[1]; Anthony J Kearsley[1]; Dmitrii V Tchekhovskoi[1]; Stephen E Stein[1]; *[1]National Institute of Standards & Technology, NIST, Gaithersburg, MD*

TP 228 **Soft-Landed Metallic Nanoparticles for Mass Spectrometry Imaging of Fingermarks**; Roberto Aguilar[1]; Guido F. Verbeck[2]; *[1]University of North Texas, Denton, TX; [2]University of North Texas, Denton, TX*

TP 229 **Automated Semi-Quantitative Screening of Benzodiazepines and Designer Benzodiazepines in Human Serum using LC-ion Trap-MS**; Ronja Peter[1, 2]; Maurice Wilde[2, 3]; Jürgen Kempf[2]; *[1]Offenburg University of Applied Sciences, Offenburg, Germany; [2]Institute of Forensic Medicine, Forensic Toxicology, Medical Center - University of Freiburg, Freiburg, Germany; [3]Hermann Staudinger Graduate School, University of Freiburg, Freiburg, Germany*

TP 230 **Separation of Isomeric Cannabinoids by High-Resolution Ion Mobility-MS for the Differentiation of Legal and Illegal Marijuana**; Marianne Hädener[1]; Marc Gonin[2]; Michael Kamrath[2]; Wolfgang Weinmann[1]; Michael Groessl[3]; *[1]University of Bern, Bern, Switzerland; [2]TOFWERK, Thun, Switzerland; [3]University Hospital Bern, Bern, Switzerland*

TP 231 **Development of an Extraction Method for Identification of a Biomarker of Sarin Exposure in Hair**; Ronald Evans[1]; Richard J Lawrence[1]; Susan L. Byers[2]; Christopher E Byers[1]; Paul Demond[2]; *[1]U.S. Army ECBC, APG-EA, MD; [2]Excet, Inc., Springfield, VA*

TP 232 **Generic Extraction Method for Screening of 8 Drugs of Abuse in Saliva with a Quick Turnaround Analysis by LDTD-MS/MS**; Sylvain Letarte[1]; Jonathan Rochon[2]; Serge Auger[3]; Jean Lacoursiere[3]; Pierre Picard[3]; *[1]Phytronix Instruments, Boisbriand, QC; [2]Universite Laval, Quebec, QC; [3]Phytronix Technologies, Quebec, QC*

TP 233 **Characterizing Exongenous Marijuana Components in Breath using a Novel Collection Device and Gas Chromatography/Mass Spectrometry**; Bruce A. Benner[1]; D'Nisha D. Hamblin[1]; Michele M. Schantz[1]; William A. MacCrehan[1]; José R. Almirall[2]; *[1]NIST, Gaithersburg, MD; [2]Florida International University, Miami, FL*

TP 234 **Comparison between High-resolution Separation and Site-specific-enzymatic Identification of Aspartic Acid and Asparagine Racemization, Isomerization, and Racemization in Eye Lens Crystallins**; Kaitlin Long[1]; Mehdi Moini[2]; *[1]George Washington University , Washington, DC; [2]George Washington University, Washington, DC*

TP 235 **Quick Identification of Uranium Compounds using Thermal Ionization Time-of-Flight Mass Spectrometry**; Dongfa Guo[1]; Zengwei Fan[1]; Guifang Liu[1]; Yuang Liu[1]; Shengkai Xie[1]; Jianyong Cui[1]; *[1]Beijing Research Institute of Uranium Geology, Beijing, China*

TP 236 **Optimization of Peptide Generation from Human Hair for Proteomic Analysis**; Zachary C Goecker[1]; Glendon J Parker[1]; Robert H Rice[1]; Michelle R Salemi[2]; Brett S Phinney[2]; *[1]University of California, Davis, Davis, CA; [2]Proteomics Core Facility, Genome Center, University of California, Davis, Davis, CA*

TP 237 **"Fowl" Odors: Identification of Blow Fly Attraction Cues in Decomposing Chicken Livers**; Justine E. Giffen[1]; Jennifer Y. Rosati[2]; Rabi A. Musah[1]; *[1]University at Albany-SUNY, Albany, NY; [2]John Jay College of Criminal Justice, New York, NY*

TP 238 **Bouquet of Death: Determination of Carrion Flower Blowfly Attractants by Ambient Mass Spectrometry**; Rabi Musah[1]; Justine E. Giffen[1]; Jennifer Y. Rosati[2]; Kristen Fowble[1]; *[1]University at Albany-SUNY, Albany, NY; [2]John Jay College of Criminal Justice, New York, NY*

TP 239 **Comparison of Screening and Quantitative LC-MS-MS Analysis of Drugs and Their Metabolites on Triple Quadrupole and Quadrupole Orbitrap Mass Spectrometers** ; Rory M Doyle[1]; Kevin McHale[1]; *[1]Thermo Fisher Scientific, Somerset, NJ*

TP 240 **LC-MSMS Analysis of Serum Samples for the Detection and Quantification of Corticosteroids in Equine Sport**; Erin Crum[1]; Jeshurun Benavides[1]; Nina Salazar[1]; Richard Sams[1]; *[1]LGC Ltd US, lexington, KY*

TP 241 **Development of Succinylcholine Chloride in Biologic Extracts using Liquid Chromatography-Tandem Mass Spectrometry**; Dai-Yong Huang[1]; Jun-Gang Lu[2]; Cai-Yong Lin[2]; Zhi-quan Yuan[2]; Shan-An Chan[3]; *[1]Agilent Technologies Ltd. Hong Kong, Hong Kong, Hong Kong; [2]Agilent Technologies (China), Guangzhou, China; [3]Agilent Technologies Inc., Taipei, Taiwan*

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TP 242 **Infrared Predissociation Spectroscopy Inside a Cryogenic Mass-Selective Trap**; Matthew Bell[1]; Nicolas C Polfer[1]; *[1]University of Florida, Department of Chemistry, Gainesville, FL*

TP 243 **IRPD Spectroscopy of Metal Cationized Ions Generated by MADLI Source: What is New?**; Xianglei Kong; *Nankai University, Tianjin*

TP 244 **Exploring Gas-Phase Structures and Properties of DNA-based Cation-Radicals with UV Action Spectra and Excited State Computations**; Andy Dang[1]; Joseph A. Korn[1]; Frantisek Turecek[1]; *[1]University of Washington, Seattle, WA*

TP 245 **Gas-Phase Conformations and N-Glycosidic Bond Stabilities of Sodium Caionized Cytosine Nucleosides: Solution Conformation of [Cyd+Na]+ is Preserved upon ESI**; Yanlong Zhu[1]; Lucas A. Hamlow[1]; Chenchen He[1]; Harrison A. Roy[1]; Nathan Cunningham[1]; Musleh Munshi[2]; Giel Berden[2]; Jos Oomens[2]; Mary T. Rodgers[1]; *[1]Wayne State University, Detroit, MI; [2]FELIX Facility, Radboud University, Netherlands*

TP 246 **Cryogenic Spectroscopy of the Protonated Serine Octamer**; Valeriu Scutelnic[1]; Marta Perez[1]; Aurelien Gregor[1]; Ursula Röthlisberger[1]; Thomas R. Rizzo[1]; *[1]EPFL, Lausanne, Switzerland*

TP 247 **A Cryogenic Linear Ion Trap for Fluorescence Spectroscopy**; Alessandra Ferzoco[1]; Vaishnavi Rajagopal[1]; *[1]Rowland Institute at Harvard, Cambridge, MA*

TP 248 **Gas-phase Infrared Spectroscopy of Proteins and Protein Assemblies**; Stephan Warnke[1]; Jongcheol Seo[2]; Waldemar Hoffmann[2]; Michael T. Bowers[3]; Kevin Pagel[4]; Gert von Helden[2]; *[1]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Berlin; [3]University of California Santa Barbara, Santa Barbara, CA; [4]Freie Universität Berlin, Berlin, Germany*

TP 249 **Characterizing Peptideβ-Hairpin Loops via Cold Ion Spectroscopy of Model Compounds**; John Thomas Lawler[1]; Christopher P Harrilal[1]; Andrew DeBlase[1]; Scott A McLuckey[1]; Timothy S Zwier[1]; *[1]Purdue University, West lafayette, Indiana*

TP 250 **Structural and Energetic Characterization of Modified Nucleosides on a Bruker amaZon ETD Quadrupole Ion Trap Mass Spectrometer**; Lucas Hamlow[1]; Yanlong Zhu[1]; Zachary Devereaux[1]; Mary T. Rodgers[1]; *[1]Wayne State University, Detroit, MI*

TP 251 **Effect of Ion Cooling in Ion Trap RF Fields**; Sergey Poteshin[1]; Anna Burykina[1]; Nikita Komar[1]; *[1]National Research Nuclear University MEPHI, Moscow, Moscow*

TP 252 **Long Distance Ion-Water Interactions in Aqueous Sulfate Nanodrops Orient Surface Water Molecules up to Tropospheric Temperatures**; Matthew J. DiTucci[1]; Christiane N. Stachl[1]; Evan R. Williams[1]; *[1]University of*

California, Berkeley, Berkeley, CA

TP 253 **Probing Conformational Isomerization and Relative Abundances between Major Conformers of 10K Gas Phase [YAP(D-Pro)AA+H]+ Ions using IR-UV Double Resonance**; Christopher Harrilal[1]; Andrew DeBlase[1]; Joshua Fischer[1]; John T Lawler[1]; Nicole L Burke[1]; Timothy S Zwier[1]; Scott A McLuckey[1]; *[1]Purdue University, West Lafayette*

TP 254 **Photodissociation Action Spectroscopy of Protonated N-containing Aromatic Ions: Can We Predict Photodissociation Pathways?**; James Bezzina[1]; Stephen J Blanksby[2]; Adam J Trevitt[1]; *[1]University of Wollongong, Wollongong, NSW; [2]Queensland University of Technology, Brisbane, Australia*

TP 255 **Reactivity and Kinetics of Ortho-substituted Phenylnitrenes**; Christopher Haskins[1]; Paul G Wenthold[1]; *[1]Purdue University, West lafayette, Indiana*

TP 256 **Energetics and Mechanism of CO2 Activation by Gadolinium Cation (Gd+)**; Maria Demireva[1]; Peter B. Armentrout[1]; *[1]University of Utah, Salt Lake City, UT*

TP 257 **Investigation on the Unimolecular and Collisional-Activated Fragmentation Mechanisms of diethyltoluidines with Isotopic Labelling Experiments**; Sarah Seulen[1]; Jurgen Grotemeyer[1]; *[1]Christian Albrechts University at Kiel, Institute for Physical Chemistry, Kiel, Germany*

TP 258 **Fragmentation Mechanisms of Azo Dye Molecules Containing Diethylamino Groups – Thermodynamic and Kinetic Considerations**; Martin Clemen[1]; Jurgen Grotemeyer[1]; *[1]Christian Albrechts University at Kiel, Institute for Physical Chemistry, Kiel, Germany*

TP 259 **The Structure of FeIII-Aerobactin Complexes: an Empirical and Theoretical Study**; Daryl Giblin[1]; Jan R Crowley[2]; Hung Tran[2]; Michael L. Gross[3]; Jeffrey P. Henderson[2]; *[1]Washington University, St Louis, MO; [2]Department of Internal Medicine, Washington University School of Medicine, St. Louis, MO; [3]Department of Chemistry, Washington University, St. Louis, MO*

TP 260 **Anionic Carbohydrate Gas-Phase Chemistry: Gelling Experimental and Theoretical Methods**; Jordan M Rabus[1]; Benjamin J Bythell[1]; *[1]University of Missouri-St. Louis, St. Louis, MO*

TP 261 **Radical-Mediated Reactions of Peptide Radical Cations: Isomerization versus Dissociation**; Xiaoyan Mu[1]; Justin Kai-Chi Lau[2, 3]; Alan C. Hopkinson[2]; Ivan K. Chu[1]; *[1]University of Hong Kong, Hong Kong; [2]York University, Toronto, ON; [3]University of Windsor, Windsor, ON*

TP 262 **Fragmentation Reactions of a7 Ions from Singly Protonated Model Heptapeptides Containing Glutamine Residue**; Ahmet Emin Atik[1]; Alex. G. Harrison[2]; Talat Yalcin[1]; *[1]Iyte, Urla-Izmir; [2]University of Toronto, Toronto, ON*

TP 263 **Gas-Phase Acidities and Conformations of Oligopeptide Epimers with D- and L-Cysteine**; Yuntao Zhang[1]; Zachary Buen[1]; Jianhua Ren[1]; *[1]University of the Pacific, Stockton, CA*

TP 264 **Investigation of the Self-Assembly Mechanism of Sandwich-Type Polyoxometalates using Mass spectrometry and X-raycrystallography**; Jie Cao[1]; Chang-Wen Hu[1]; Lin-Yuan Fan[1]; *[1]Beijing Institute of Technology, Beijing, China*

TP 265 **Fragmentation and H/D Exchange Studies of Tetrapeptides Containing Lysine Homologues**; Melanie A Berger[1]; Zachariah I. Hasan[1]; Anna Do[1]; Danielle A. Long[1]; Anwar Radwan[1]; John Poutsma[1]; *[1]College of William & Mary, Williamsburg, VA*

TP 266 **IRMPD Studies of b2 and b3 Ions From Lysine Analog-Containing Peptides**; Zachary M. Smith[1]; Vincent Steinmetz[2]; Arpad Somogyi[3]; Vicki H. Wysocki[3]; John Poutsma[1]; *[1]College of William & Mary, Williamsburg, VA; [2]Universite de Paris Sud, Orsay, France; [3]Ohio State University, Columbus, OH*

TP 267 **Role of Residual Water Molecules into a Linear Ion Trap Cell on Re-Orientation of Aspartate and Glutamate Anion Dissociations**; Pierre Barbier Saint Hilaire[1]; Yves Gimbert[2]; Anna Warnet[1]; Annelaure Damont[1]; Marie-Françoise Olivier[1]; Benoit Colsch[1]; François Fenaille[1]; Christophe Junot[1]; Jean-Claude Tabet[1, 3]; *[1]CEA, iBiTecS, SPI, Laboratoire d'Etude du Métabolisme des Médicaments, MetaboHUB-Paris, Université Paris Saclay, Gif-sur-Yvette cedex, France; [2]Université Grenoble Alpes (DCM), CNRS-UJF 5250, BP 38041, Grenoble, France; [3]Sorbonne Universités, UPMC Univ Paris 06, CNRS, Institut Parisien de Chimie Moléculaire (IPCM), Paris, France*

TP 268 **An Ion Mobility Database of Metal-Coordinated Peptide Ions: General Structural Effects upon Alkali, Alkaline-earth, or Transition-metal Interaction**; Jonathan Dilger[1]; David E Clemmer[2]; *[1]Naval Surface Warfare Center, Crane Division, Crane, IN; [2]Indiana University Bloomington, Bloomington, IN*

TP 269 **Size-selective Anion Binding by Cucurbit[5]uril Characterized Using SORI-CID Techniques**; Jiewen Shen[1]; David V. Dearden[2]; *[1]Brigham Young University, Provo, UT; [2]Brigham Young University, Provo, UT*

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TP 270 **Chemometric Methods for Analysis of Graftage-related Black Tea Aroma Variation by Solid Phase Mirco-extraction and Gas Chromatography-Mass Spectrometry**; Wei Chen[1]; Wenwen Wang[2]; Chengying Ma[1]; Junxi Cao[1]; Aiqing Miao[1]; Shi Pang[1]; *[1]Tea Research Institute, Guangdong Academy of Agricultural Sciences, Guangzhou, China; [2]Agilent Technologies (China), Beijing, China*

TP 271 **Atmospheric Pressure Gas Chromatography/Mass Spectrometry for the Analysis of Organochlorine Pesticides, Polychlorinated Biphenyls and Polybrominated Diphenyl Ethers in Human Serum**; Jing Fang[1]; Xiubao Huang[1]; Yanhao Zhang[1]; Hongzhi Zhao[1]; Zongwei Cai[1]; *[1]State Key Laboratory of Environmental and Biological Analysis, Department of Chemistry, Hong Kong Baptist University, Hong Kong, Hong Kong*

TP 272 **Simultaneous Determination of 12 Tobacco Alkaloids inE-liquids for Electronic CigarettesUsing Gas Chromatography - Mass Spectrometry Method**; Shulei Han[1]; Yaning Fu[1]; Tong Liu[1]; Huan Chen[1]; Hongwei Hou[1]; Qingyuan Hu[1]; *[1]China National Tobacco Quality Supervision & Test Centre, Zhengzhou, China*

TP 273 **Determination of Fatty Acid Esters of 2- and 3-monochloro-1,2-propanediol (MCPD) and Glycidol in Edible Oil Using GC-Triple Quadrupole Mass Spectrometry**; Samuel Chao Ming Yeo[1]; Crystal Hui Xian Yeong[1]; Kok Ming Goh[2]; Chin Pang Tan[2]; May Yen Ang[3]; Lai Chin Loo[1]; *[1]Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore; [2]Department of Food Technology, Faculty of Food Science and Technology, Universiti Putra Malaysi, 43400 UPM Serdang, Malaysia; [3]Shimadzu Malaysia Sdn Bhd, Taman Sains Selangor I, Malaysia*

TP 274 **Quantifying Flavorings in E-cigarette Aerosol as a Function of Power Applied to the Heating Coil**; Nicholas Wallbillich[1]; Gary Glish[2]; *[1]UNC, Chapel Hill, NC; [2]Professor, Chapel Hill, North Carolina*

TP 275 **Analysis of Cannabidiols found in Cannabis by Thermal Desorption GC/MS**; Ronald Shomo[1]; Christopher Baker[1]; john manura[1]; *[1]Scientific Instrument Services, Ringoes, NJ*

TP 276 **Diagnostically Important Ions in Mass Spectra of Silyl, Sulfonyl, Alkoxycarbonyl and Perfluoroacyl Derivatives of Substituted Phenols**; Nino G. Todua[1]; Levan A. Megutnishvili[2]; Anzor I. Mikaia[2]; *[1]NIST / Dakota C., Gaithersburg, MD; [2]NIST, Gaithersburg, MD*

TP 277 **Integrated Microextraction, Syringe Headspace, and**

SPME Characterization of Organic Contamination from Plastic Bags by GC/MS; Adam J. Patkin [1]; Charlie Schmidt[1]; *[1]PerkinElmer, Shelton , CT*

TP 278 **Off-flavour Analysis in Food Using a Simple and Rapid Solid Phase Microextraction-GC/Triple Quadrupole Mass Spectrometry Method with Dedicated Off-flavour Database**; Samuel Chao Ming Yeo[1]; Cynthia Melanie Lahey[1]; Lai Chin Loo[1]; *[1]Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore*

TP 279 **Qualitative Profiling of Co-polymer Polyethylene Terephthalate through Multifunctional Pyrolyzer-GC/MS by various Thermal Treatment Techniques**; Guo Wei Elgin Ting[1]; Stephany Olivia[2]; Chiang Yong Douglas Chong[3]; Hui Xian Crystal Yeong[1]; Lai Chin Loo[1]; *[1]Application Development & Support Centre, Shimadzu (Asia Pacific) Pte Ltd, Cintech IV, Singapore Science Park, Singapore; [2]Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore; [3]Department of Chemistry, Faculty of Science, National University of Singapore, Singapore*

TP 280 **Analysis of Fast Moving Consumer Goods (FMCG) using GCMS with Static and Dynamic Headspace (HS)**; Dheeraj Handique[1]; Ankush Bhone[1]; Prashant Hase[1]; Sanket Chiplunkar[1]; Durvesh Sawant[1]; Nitish Suryawanshi[1]; Ajit Datar[1]; Jitendra Kelkar[1]; Pratap Rasam[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

TP 281 **Addressing the Challenges of Short Chained Chlorinated Paraffins Analysis using Orbitrap GC-MS**; Cristian Cojocariu[1]; Paul Silcock[2]; *[1]Thermo Fisher Scientific, Runcorn, UK; [2]Thermo Fisher Scientific, Runcorn, Cheshire*

TP 282 **Characterization of Perfumes via Tandem Vacuum Ultraviolet Spectroscopy and Mass Spectrometry**; Ian Anthony[1]; Adam R. Floyd[1]; Christina A. Gaw[1]; Matthew R. Brantley[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, Texas*

TP 283 **Fluorine Tagging for Quantification of Krebs Cycle Metabolites using Gas-Chromatography Plasma Assisted Reaction Chemical Ionization Mass Spectrometry**; Michael Dolan[1]; Kunyu Zheng[2]; Steven Peyton[3]; Amrita Cheema[3]; Kaveh Jorabchi[2]; *[1]Georgetown University, Washington, DC; [2]Georgetown University, Washington, DC; [3]Georgetown University Medical School, Washington, DC*

TP 284 **Loss of SO2 from o-Nitro Substituted Diaryl Sulfides and Related Compounds**; Yufang Zheng[1]; Quanlong Pu[2]; Edward White V[2]; Stephen E. Stein[2]; *[1]NIST / Dakota C., Gaithersburg, MD; [2]NIST, Gaithersburg, MD*

TP 285 **Method for Determining Kinetic Parameters of Chemical Warfare Nerve Agent Decomposition via Pyrolysis GC-MS**; Jeffrey Michael Mcguire[1]; John C Carpin[1]; William T Muse[1]; *[1]US Army ECBC, Aberdeen Proving Ground, MD*

TP 286 **Analysis of Modified Graphene Oxidenanomaterial using STA/FT-IR/GC-MS**; Xiaoying Yan[1]; Zhuo Man[2]; Xiangdong Zhou[2]; Jason Weisenseel[3]; Yong-Ming Xie[2]; *[1]National Center for Nanoscience and Technology, Beijing, China; [2]PerkinElmer Management (Shanghai) Co, Shanghai, China; [3]PerkinElmer, Shelton , CT*

TP 287 **Analysis of Unknown Contaminants in Interior Air Spray using TGA/FT-IR/GC-MS**; Fei Zhang[1]; Zhuo Man[2]; Xiangdong Zhou[2]; Desmond Wichems[3]; Yongming Xie[2]; *[1]Peking University, Beijing, Beijing; [2]PerkinElmer Management (Shanghai) Co, Shanghai, China; [3]PerkinElmer Inc., San Jose, CA*

TP 288 **Evaluation of select-eV, two-dimensional-GC and Large Volume Injection on the Limits of Detection and Quantification of Cannabinoids in Hair Samples**; Emma Beasley[1]; Geraint Morgan[2]; Tom Bassindale[1]; *[1]Sheffield Hallam University, Sheffield, UK; [2]The Open University, Milton Keynes, UK*

TP 289 **Headspace Solid Phase Micro-Extraction (HS-SPME) of Volatile Compounds Encapsulated in Flash Frozen Coffee Extracts**; Mary Elizabeth Gimon-Kinsel[1]; Jackson Frazier Wood[1]; *[1]Southern Illinois University, Carbondale, IL*

TP 290 **Identification of Salivary Metabolomics Biomarkers of Chronic Kidney Disease and Their Association with Periodontitis**; Levy Alves[1, 2, 3, 4]; Rafael Celestino Souza[3]; Taciana Mara Couto da Silva Mara Couto da Silva[3]; Meriellen Dias[2, 5]; Deise Garrido[3, 5]; maria anita mendes[2, 5]; Ana Lidia Ciamponi[3, 5]; *[1]Guarulhos University, São Paulo, SP; [2]Dempster Mass Lab- POLI- USP, Sao Paulo, Brazil; [3]Dental School of USP, São Paulo, Brazil; [4]Paulista University, São Paulo, Brazil; [5]Universidade de São Paulo - USP, Sao Paulo, South America*

TP 291 **Evaluation of a High-Sensitivity GC-MS/MS in the Analysis of Pesticide Residues in Complex Samples: Cost Savings and Other Benefits**; Katerina Mastovska[1]; Lukas Vaclavik[2]; Melissa Churley[3]; Thomas P. Doherty[3]; *[1]Covance, Madison, WI; [2]Covance, Harrogate, UK; [3]Agilent Technologies, Inc., Santa Clara, CA*

TP 292 **Applying Pyrolysis GC/MS to the Characterization of Agricultural Formulations**; Todd Kajdan; *Dow AgroSciences, Indianapolis, IN*

TP 293 **GCMS and NMR Based Chemometrics of Distillates**; Mary Jean Riches[1]; Kaylen Obray[1]; Karolien Denef[1]; Claudia Boot[1]; Chris Rithner[1]; *[1]Colorado State University, Fort Collins, CO*

TP 294 **Determination of Retention Indices of Organic Compounds in Comprehensive Two-Dimensional Gas Chromatography-Mass Spectrometry (GCxGC-MS)**; Dmitrii Mazur[1]; Olga Polyakova[1]; Albert Lebedev[1]; *[1]M.V. Lomonosov Moscow State University, Moscow, Russia*

TP 295 **Fast Screening and Quantitation of Perfluorinated Sources from Textiles Using Gas Chromatography Chemical Ionization Mass Spectrometry**; Hui Xian Crystal Yeong[1]; Stephany Olivia[2]; Lai Chin Loo[1]; *[1]Application Development & Support Centre, Shimadzu (Asia Pacific) Pte Ltd, 79 Science Park Drive, #02-01/08, Cintech IV, Singapore Science Park 1, Singapore 118264, Singapore, Singapore; [2]Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University, 21 Nanyang Link SPMS-04-01, Singapore 627371, Singapore, Singapore*

TP 296 **Fast and Accurate Quantitation of Perfluorinated Sources from Textiles Using Gas Chromatography-Triple Quadrupole Mass Spectrometry**; Hui Xian Crystal Yeong[1]; Stephany Olivia[2]; Cynthia Melanie Lahey[1]; Guo Wei Elgin Ting[1]; Lai Chin Loo[1]; *[1]Application Development & Support Centre, Shimadzu (Asia Pacific) Pte Ltd, 79 Science Park Drive, #02-01/08, Cintech IV, Singapore Science Park 1, Singapore 118264, Singapore, Singapore; [2]Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University, 21 Nanyang Link SPMS-04-01, Singapore 627371, Singapore, Singapore*

TP 297 **Determination of Cannabinoids from a Surrogate Hops Matrix Using Multiple Reaction Monitoring Gas Chromatography – Triple Quadrupole – Mass Spectrometry**; Allegra Leghissa[1]; Kevin A. Schug[2]; *[1]University Of Texas, Arlington, Arlington, TX; [2]University of Texas, Arlington, Arlington, TX*

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TP 298 **A Method for the Quantitative Monitoring of Site-Specific Glycosylation of Proteins in Large Sample Set Analysis**; Elisha Goonatilleke[1]; Jincui Huang[1]; Lauren Dimapasoc Wu[1]; Gege Xu[1]; Carlito B Lebrilla[1]; *[1]University of California, Davis, Davis, CA*

TP 299 **Site-Specific Fucosylation Analysis of Glycoproteins**

from Aggressive Prostate Cancer Cells Using Affinity Enrichments of Intact Glycopeptides Followed by Mass Spectrometry; Jianliang Zhou[1]; Weiming Yang[1]; Yingwei Hu[1]; Naseruddin Hoti[1]; Punit Shah[1]; Hui Zhang[1]; *[1]Johns Hopkins University School of Medicine, Baltimore, MD*

TP 300 **Comparison of Site-Specific N-Glycoproteins between Human and Mouse Plasma Using LC-MS/MS and Database Search**; Juyeon Lee[1, 2]; Hyun Kyoung Lee[1, 3]; Gun Wook Park[1]; Kun Cho[1, 2]; Jeong Gu Kang[2]; Yong-Sam Kim[2]; Jeong-Heon Ko[2]; Jin Young Kim[1]; Jong Shin Yoo[1]; *[1]Korea Basic Science Institute, 162 YeonGuDanji-Ro, Ochang-eup, Cheongwon-gu, Cheongju, South Korea; [2]Korea Institute of Bioscience and Biotechnology, Daejeon, South Korea; [3]Graduate School of Analytical Science and Technology, Daejeon, South Korea*

TP 301 **Glycosylation Analysis of Spike Protein from Infectious Bronchitis Viruses with Different Tissue Binding Properties**; Lisa Parsons[1]; Kim Bouwman[2]; Helene Verheije[2]; John F Cipollo[1]; *[1]FDA, Silver Spring, MD; [2]Utrecht University, Utrecht, Netherlands*

TP 302 **Glycoproteomics Analysis to Examine the Role of Chlamydial Protease-Like Activity Factor**; Christa Feasley[1]; Fred Zinnel[2]; Julian Saba[3]; Stuart McCorrister[4]; Garrett Westmacott[4]; Grant McClarty[4]; Chris Grant[4]; *[1]Thermo Fisher Scientific, West Palm Beach, Florida; [2]Thermo Fisher Scientific, Somerset, NJ; [3]Thermo Fisher Scientific, Mississauga, Ontario; [4]National Microbiology Laboratory, Public Health Agency of Canada, Winnipeg, MB*

TP 303 **Glycoproteomic Analysis of Temozolemide-Resistant Glioma Cells by MALDI-TOF/TOF MS and nano-HPLC-QTOF-MS/MS**; Milan Teraiya[1]; Emy Komatsu[1]; Jenna Noordenbos[2]; Helene Perreault[3]; Vincent C Chen[2]; *[1]University of Manitoba, Winnipeg, MB; [2]Brandon University, Department of Chemistry, Brandon, MB; [3]University of Manitoba, Winnipeg, MB*

TP 304 **Global Analysis of Secreted N-Glycoproteins in MCF7 Cells Using Click Chemistry-Based Enrichment and Mass Spectrometry**; Fangxu Sun[1]; Haopeng Xiao[1]; Ronghu Wu[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

TP 305 **Quantitative Analysis of N- and O- Glycans from Cerebrospinal Fluid in Alzheimer's Disease Patients**; Byeong G. Cho[1]; Aiying Yu[1]; Lucas Veillon[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

TP 306 **Site-Specific Characterization and Quantitation of N-Glycoproteins in Breast Cancer Cells Using DiLeu Isobaric Tags Enabled by Electron-Transfer/Higher-Energy Collision Dissociation (EThcD)**; Zhengwei Chen[1]; Qing Yu[1]; Ling Hao[1]; Fabao Liu[1]; Jill Johnson[1]; Zichuan Tian[1]; Wei Xu[1]; Lingjun Li[1]; *[1]University of Wisconsin Madison, Madison, WI*

TP 307 **Systematic Investigation of Glycan Maturity on Human Cell Surface Glycoproteins**; Suttipong Suttapitugsakul[1]; Johanna Smeekens[1]; Haopeng Xiao[1]; Ronghu Wu[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

TP 308 **Mass Spectrometry-Based Characterization of Recombinant Human Immunodeficiency Virus Type 1 (HIV-1) Envelope (Env) Glycoprotein**; Vaneet Kumar Sharma; *International AIDS Vaccine Initiative (IAVI), New York, NY*

TP 309 **An Insight into Glyco-microheterogeneity of Plasma von Willebrand Factor (vWF) by MS Spectrometry**; Ebtesam Gashash[1, 2]; Arya Aloor[1]; He Zhu[1]; Cong Xiao[1]; Ding Liu[1]; Jing Song[1]; Cheng Ma[1]; Weidong Xiao[3]; Peng Wang[1]; *[1]GSU, Atlanta, GA; [2]Albaha University, Baljurashi, Saudi Arabia; [3]Sol Sherry Thrombosis Research Center, Temple University, Philadelpha, PA 19140*

TP 310 **A Novel Method Combining Enzymatic and Chemical Reactions to Identify Glycoproteins with the Tn Antigen**; Jiangnan Zheng[1]; Haopeng Xiao[1]; Ronghu Wu[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

TP 311 **Effects of Illiciting Immune Response in Rabbits on IgG N-Glycans**; Tyler Fletcher[1]; Ron Orlando[1]; *[1]University of Georgia, Athens, GA*

TP 312 **Glycan Heterogeneity Differentiation Using Lectin-Based SDC Separation and Glycopeptide level SDC Separation**; Wonryeon Cho; *Wonkwang University, Iksan, Jeonbuk*

TP 313 **Assisting the Characterization of IgG Glycosylation with a Hydrophilic Interaction Liquid Chromatography Retention Model for Glycopeptides**; Emily Betchy[1]; Barry Boyes[2]; Ron Orlando[1]; *[1]CCRC, University of Georgia, Athens, GA; [2]Advanced Materials Technology, Wilmington, DE*

TP 314 **Characterization of Glycan Structures of Zika Virus**; Zhichao Zhang[1]; Christopher Brown[2]; Yixiang zhang[2]; David E Clemmer[2]; *[1]Indiana University, Bloomington, IN; [2]Indiana University Bloomington, Bloomington, IN*

TP 315 **Comparative Glyomic Approaches for Assessment of Glycosylation in a Therapeutic Glycoprotein**; Nayoung Yun[1, 2]; Nari Seo[2, 3]; Unyong Kim[2]; Myung Jin Oh[2, 3]; Hyun Joo An[2, 3]; *[1]Chungnam National University, Daejeon, Chungcheongnam; [2]Asia Glycomics Reference Site, Daejeon, South Korea; [3]Chungnam National University, Daejeon, South Korea*

TP 316 **Workflows for the Identification and Relative Quantitation of Glycan Variants**; Stephen Madden[1]; Aaron Boice[1]; Aditi Koul[1]; Caroline S. Chu[1]; *[1]Agilent Technologies, Inc., Santa Clara, CA*

TP 317 **Identification of Glycoprotein Biomarkers for Hepatocellular Carcinoma**; Cristina Di Poto[1]; Minkun Wang[1]; Shan Su[1]; Junfeng Ma[1]; Habtom W. Ressom[1]; *[1]Georgetown University, Lombardi Cancer Center, Washington, DC*

TP 318 **Glycoproteomic Identification and Quantification of Human Plasma with IQ-GPA and Database Search**; Gun Wook Park[1]; Ju Young Kim[1]; Ju Yeon Lee[1]; Heeyoun Hwang[1]; Hyun Kyoung Lee[1]; Eun Sun Ji[1]; Kwang Hoe Kim[1, 2]; Hoi Keun Jeong[1, 2]; Ki Na Yun[1, 3]; Yong-Sam Kim[4]; Jeong-Heon Ko[4]; Jong Shin Yoo[1, 2]; *[1]Biomedical Omics Group, Korea Basic Science Institute, Cheongju-si, South Korea; [2]Graduate School of Analytical Science and Technology, Chungnam National University, South Korea; [3]Department of Chemistry, Sogang University, 35 Baekbeom-ro, Mapo-gu, South Korea; [4]Cancer Biomarkers Development Research Center, Korea Research Institute of Bioscience and Biotechnology, Daejeon, South Korea*

TP 319 **Global and Site-Specific Analysis Reveals Unexpected and Extensive Protein S-GlcNAcylation in Human Cells**; Haopeng Xiao[1]; Ronghu Wu[1]; *[1]Georgia Tech , Atlanta, GA*

TP 320 **New Analytical Platform to Explore Haptoglobin Glycosylation Using Intact Glycoprotein**; Unyong Kim[1, 2]; Hantae Moon[1, 2]; Sung Hyun Lee[3]; Myung Jin Oh[1, 2]; Jua Lee[1, 2]; Seung Hyup Jeong[1, 2]; Hyun Joo An[1, 2]; *[1]Asia Glycomics Reference Site, Chungnam National University, South Korea; [2]Chung Nam Univ., Daejeon; [3]Glycan Inc., Seongnam-si, South Korea*

TP 321 **Mass Spectrometry Analysis of Platelet Glycome Using Intact Glycopeptides Analysis Approach**; Punit Shah[1]; Hui Zhang[1]; *[1]Johns Hopkins University, Baltimore, MD*

TP 322 **An O-Glycosylated Archaeal Flagellin Extensively Adorned with Two Unusual Saccharides**; Hong Hanh Nguyen[1]; Nicole Poweleit[1]; Deborah Leon[2]; Catherine E. Costello[2]; Joseph A Loo[1]; Robert P. Gunsalus[1]; Rachel R. Ogorzalek Loo[1]; *[1]UCLA, Los Angeles, California; [2]Boston University, Boston, MA*

TP 323 **Mapping Site-Specific N-Glycosylation of B-Cell Receptor in B-Cell Lymphomas**; Kuan-Ting Pan[1]; Carmen Doebele[2]; Kay-Hooi Khoo[3]; Thomas Oellerich[4, 5, 6]; Henning Urlaub[1, 7]; *[1]Bioanalytical Mass Spectrometry, MPI for Biophysical Chemistry, Goettingen, Germany; [2]Department of Hematology/Oncology, Johann Wolfgang*

Goethe University, Frankfurt am Main, Germany; [3]Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan; [4]Department of Hematology/Oncology, Johann Wolfgan Goethe University, Frankfurt am Main, Germany; [5]German Cancer Research Center (DKFZ), Heidelberg, Germany; [6]Department of Haematology, University of Cambridge, Cambridge, UK; [7]Bioanalytics, Department of Clinical Chemistry, University Medical Center Goettingen, Goettingen, Germany

TP 324 **Site-Specific and Structural Analysis of Protein O-Mannosylation in *Saccharomyces cerevisiae***; Haopeng Xiao[1]; Ronghu Wu[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

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TP 325 **Imaging Mass Spectrometry of Image-Guided Drug Delivery (IGDD) in Thermochemical Ablation**; Chunxiao Guo[1]; Dodge Baluya[1]; Rick Layman[1]; Erik Cressman[1]; *[1]MD Anderson, Houston, TX*

TP 326 **Visualizing Chemical Communication Governing Metastasis of Ovarian Cancer with Imaging Mass Spectrometry**; Katherine Zink[1]; Joanna E Burdette[2]; Matthew Dean[2]; Laura M Sanchez[2]; *[1], Chicago, IL; [2]University of Illinois at Chicago, Chicago, Illinois*

TP 327 **Feasibility Studies in Imaging Mass Spectrometry for Evaluating Thermoembolization, a New Interventional Oncologic Technique**; Chunxiao Guo[1]; Dodge Baluya[1]; Rick Layman[1]; Erik Cressman[1]; *[1]MD Anderson, Houston, TX*

TP 328 **Liquid Chromatography-Mass Spectrometry-Based Metabolomics and Lipidomics Reveal Toxicological Mechanism of Bisphenol F in Breast Cancer Xenografts**; Chao Zhao[1, 2]; Peisi Xie[3]; Yuanyuan Song[1]; Ti Yang[1]; Zhi Tang[1]; Hailin Wang[2]; Zongwei Cai[1]; *[1]state Key Laboratory of Environmental and Biological Analysis, Department of Chemistry, Hong Kong Baptist University, Hong Kong SAR, China; [2]State Key Laboratory of Environmental Chemistry and Ecotoxicology, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing, China; [3]Ministry of Education Key Laboratory of Analysis and Detection Technology for Food Safety, Fuzhou University, Fuzhou, China*

TP 329 **Multiscale Mass Spectrometry Imaging of Colorectal Cancers by MALDI, DESI and SIMS**; Rory T Steven[1]; Adam J Taylor[1]; Spencer A Thomas[1]; Alan M Race[1]; Gregory Hamm[2]; Nicole Strittmatter[2]; Rasmus Havelund[1]; Renata F Soares[3]; Andrew D Campbell[4]; Owen J Sansom[4]; Richard J. A. Goodwin[5]; Zoltan Takats[3]; Josephine Bunch[1]; *[1]National Physical Laboratory, Teddington, UK; [2]AstraZeneca R&D, Cambridge, UK; [3]Imperial College London, London, London; [4]Beatson Institute for Cancer Research, Bearsden, UK; [5]Astrazeneca, Cambridge, UK*

TP 330 **Mass Spectrometric Analysis of Endogenous Small Molecules and Chemotherapeutic Doxorubicin in a Three-Dimensional Cell Culture Model of Osteosarcoma**; Ieva Palubeckaite[1]; Neil Cross[1]; Christine Le Maitre[1]; David Smith[1]; Chris Sammon[1]; Malcolm Clench[1]; *[1]Sheffield Hallam University, Sheffield, UK*

TP 331 **Technical Challenges of Mass Spectrometry Imaging of Doxorubicin Localization in Rat Liver Treated with Drug-Eluting Beads**; Dodge Baluya[1]; Andrea Cortes[1]; Hideyuki Nishiofuku[1]; Rony Avritscher[1]; Erik Cressman[2]; *[1]MD Anderson Cancer Center, Houston, TX; [2]MD Anderson, Houston, TX*

TP 332 **Gold Nanoparticles as MALDI MSI Matrix for Imatinib Distribution and Quantitation Analysis Inside Tumor Tissues**; Silvia Giordano[1]; Lavinia Morosi[1]; Francesca Falcetta[1]; Mridula Prasad[2]; Ilaria Fuso Nerini[1]; Simonetta Andrea Licandro[1]; Roberta Frapolli[1]; Paolo Ubezio[1]; Maurizio D'Incalci[1]; Massimo Zucchetti[1]; Pietro Franceschi[2]; Sonja Visentin[3]; Enrico Davoli[1]; *[1]Mario Negri Institute, Milano; [2]Fondazione E.Mach, San Michele all'Adige, Italy; [3]University of Torino, Turin, Italy*

TP 333 **Mapping the Brain Neurotransmitter Network with MALDI MS Imaging**; Mohammadreza Shariatgorji[1]; Luke Odell[1]; Anna Nilsson[1]; Elva Fridjonsdottir[1]; Luay Katan[1]; Jonas Sävmarker[1]; Matthias Witt[2]; Per Svenningsson[3]; Per E. Andren[1]; *[1]Uppsala University, Uppsala, SE; [2]Bruker Daltonics, Bremen, Germany; [3]Karolinska Institutet, Stockholm, Sweden*

TP 334 **Matrix Assisted Laser Desorption Ionization Imaging Mass Spectrometry of Human Osteoarthritis Cartilage Reveals the Intra-Tissue Metabolic Heterogeneity**; Maxime Eveque-Mourroux[1, 2, 3]; Pieter Emans[2]; Tim Welting[2]; Annelies Boonen[3]; Ron Heeren[1]; Berta Cillero-Pastor[1]; *[1]Maastricht Multi-Modal Molecular Imaging (M4I) Institute, Maastricht University, Maastricht, Netherlands; [2]Maastricht University Medical Center, Department of Orthopedic Surgery, Maastricht, Netherlands; [3]Maastricht University Medical Center, Caphri Research institute, Maastricht, Netherlands*

TP 335 **Visualizing NMF Distribution across the Human Face by 2D-DESI MS Imaging of Tape-Stripped Stratum Corneum**; Keishi Kihara[1]; Akira Motoyama[1]; *[1]Shiseido Co., LTD., Yokohama, Kanagawa*

TP 336 ***Pseudomonas aeruginosashifts* its Specialized Metabolism in Response to Biofilm Inhibitors.**; Alanna Condren[1]; Laura M. Sanchez[1]; *[1]University of Illinois, Chicago, Illinois*

TP 337 **Analyzing Liposomal Drug Delivery Systems in Three-Dimensional Cell Culture Models Using MALDI-Imaging Mass Spectrometry and Fluorescence Microscopy**; Jessica K. Lukowski[1]; Eric M. Weaver[2]; Amanda B. Hummon[2]; *[1], Notre Dame, IN; [2]University of Notre Dame, Notre Dame, IN*

TP 338 **MALDI Imaging of Lipase Activity on Textile Surfaces**; Jonatan Hall-Andersen[1]; Svend G. Kaasgaard[2]; Christian Janfelt[1]; *[1]University of Copenhagen, Copenhagen, Denmark; [2]Novozymes A/S, Bagsvaerd, Denmark*

TP 339 **Demonstrating the Applicability of DESI Imaging Coupled with Ion Mobility for Mapping Cosmetic Ingredients on Tape Stripped Skin Samples**; Eleanor Riches[1]; Oliver O. Burt[1]; Philippa J. Hart[1]; Emmanuelle Claude[1]; Malcolm R. Clench[2]; *[1]Waters Corporation, Wilmslow, UK; [2]Spectrometry Imaging, Biomolecular Sciences Research Centre, Sheffield Hallam University, Howard Street, Sheffield, UK*

TP 340 **Laden Latents: Revealing Human Handling of Psychoactive Plant Materials through Biomarker Fingerprint Imaging by MALDI-SpiralTOF High-Resolution Mass Spectrometry**; Cameron M. Longo[1]; Rabi A. Musah[1]; *[1]University at Albany-SUNY, Albany, NY*

TP 341 **Mass Spectrometry Imaging of Neurotransmitters in Brain Tissue after Intake of Drugs of Abuse**; Ludovic Muller[1]; Shelley N. Jackson[1]; Amina S. Woods[1]; *[1]NIH/NIDA-IRP, Baltimore, MD*

TP 342 **Mass Spectrometry Imaging of Small Xenobiotics on *Danio rerio* : Influence of Molecular Profiles Modification as Potential Localization Asset.**; Mathieu Tiquet[1]; Marc Muller[2]; Edwin De Pauw[1]; *[1]Mass Spectrometry Laboratory, Liège, Belgium; [2]GIGA-R : Biologie et génétique moléculaire, Liège, Belgium*

TP 343 **Optimizing Physical Properties of Formulations Using LAESI Mass Spectrometry**; Suresh Annangudi[1]; Erin Gemperline[2]; Gary Gustafson[2]; Kyung Myung[2]; Jeffrey Gilbert[2]; Steve Wilson[2]; *[1]Dow Agrosciences, Indianapolis, IN; [2]Dow AgroSciences, Indianapolis, IN*

TP 344 **Localisation of Caffeoyl Quinates in Developing**

Beans of Robusta Coffee (*Coffea canephora*) ; Gerhard Saalbach[1]; Cathie Martin[1]; James McCarthy[2]; Daniel Knevitt[1]; *[1]John Innes Centre, Norwich, Norfolk; [2]Nestlé Research and Development Center Tours France, Tours, France*

TP 345 **Visualization of Abscisic Acid and 12-Oxo-Phytodienoic Acid in Immature *Phaseolus vulgaris* L. Seeds Using Desorption Electrospray Ionization-Imaging Mass Spectrometry**; Hirofumi Enomoto[1]; Takuya Sensu[1]; Futoshi Sato[2]; Emi Yumoto[1]; Takao Yokota[1]; Hisakazu Yamane[1]; *[1]Department of Biosciences, Faculty of Science and Engineering, Teikyo University, Utsunomiya, Japan; [2]Waters Corporation, Shinagawa, Japan*

TP 346 **Matrix–Assisted Laser Desorption/Ionization-Mass Spectrometry Imaging (MALDI-MSI) for Direct Visualization of Wheat Grain Metabolites**; Shabarinath Nambiar[1]; Robert Trengove [1]; Sze How Bong[1]; Joel Gummer[1]; *[1]Murdoch University, Murdoch , WA*

TP 347 **GCIB-ToF-SIMS High Resolution Imaging of Cardiolipin Speciation in the Brain: Identification of Molecular Losses after Traumatic Injury**; L.J. Sparvero[1]; Hua Tian[2]; Andrew A Amoscato[1]; Anna Bloom[2]; Nicholas Winograd[2]; Valerian E Kagan[1]; Hülya Bayır[1]; *[1]University of Pittsburgh, Pittsburgh, PA; [2]Pennsylvania State University, State College, PA*

TP 348 **Comparative Tissue Imaging for Disease Characterization Using DESI Coupled with Uniform Field Drift Tube Ion Mobility High Resolution Mass Spectrometry**; Ruwan T Kurulugama[1]; Joseph H Kennedy[2]; Brian C Laughlin[2]; Justin M Wiseman[2]; George Stafford[1]; John Fjeldsted[1]; *[1]Agilent Technologies Inc., Santa Clara, California; [2]Prosolia Inc., Indianapolis, IN*

TP 349 **Comparison of Laser Ablation Atmospheric Pressure Photoionization (LAAPPI) and Laser Ablation Electrospray Ionization (LAESI) in MS Imaging of Animal Tissue**; Juha-Pekka Hieta[1]; Anu Vaikkinen[1]; Heikki Räikkönen[1]; Jaakko Kopra[1]; Petteri Piepponen[1]; Markus Haapala[1]; Tiina J. Kauppila[1]; *[1]University of Helsinki, Helsinki, Finland*

TP 350 **Spatial Mapping of Metabolites and Neurotransmitter in Rat Brain Sections Using DESI Ion Mobility Mass Spectrometry**; Anthony J. Midey[1]; Hernando J. Olivos[1]; Michael Batey[2]; Emmanuelle Claude[2]; Bindesh Shrestha[3]; *[1]Waters Corporation, Beverly, MA; [2]Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK; [3]Waters Corp., Beverly, MA*

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TP 351 **Crosstalker: An Open and Flexible Network and Pathway Analysis Platform**; Sean Maxwell[1, 2]; Mark R. Chance[1, 2]; *[1]Center for Proteomics and Bioinformatics, Case Western Reserve University, Cleveland, OH; [2]Department of Nutrition, Case Western Reserve University, Cleveland, OH*

TP 352 **Multiomics Data Integration Using Anatomical Ontologies**; Magnus Palmblad; *Leiden University Medical Center, Leiden, Netherlands*

TP 353 **Proteogenomics Reveals a Complicated Feature of the Molecular Characteristics of Colorectal Cancer in AOM/DSS Mouse Model**; Qingfei Pan[1, 2]; Yingying Xie[1]; Lylia Drici[3]; Yanxia Liu[1]; Lei Sun[1]; Honggang Huang[3]; Bo Wen[2]; Martin Røssel Larsen[3]; Xiaomin Lou[1]; Yan Ren[2]; Lin Wu[1]; Peter Roepstorff[3]; Siqi Liu[1, 2]; *[1]Beijing Institute of Genomics, Chinese Academy of Sciences, Beijing, China; [2]BGI-Shenzhen, Shenzhen, China; [3]Protein Research Group, Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense, Denmark*

TP 354 **Proteogenomics of Adenosine-to-Inosine RNA Editing in Fruit Fly**; Ksenia G Kuznetsova[1]; Irina Y Ilina[1]; Alexey L Chernobrovkin[2]; Svetlana E Novikova[1]; Tatyana E Farafonova[1]; Dmitry S Karpov[3]; Mark I Ivanov[4, 5]; Olga E Voronko[1]; Victor G Zgoda[1]; Roman A Zubarev[2]; Mikhail V Gorshkov[4, 5]; Sergei A Moshkovskii[1, 6]; *[1]Institute of Biomedical Chemistry, Moscow, Russia; [2]Karolinska Institute, Stockholm , Uppland; [3]Engelhardt Institute of Molecular Biology, Moscow, Russia; [4]Institute of energy problems of chemical physics Russian Academy of Sciences, Moscow, Russia; [5]Moscow institute of physics and technology, Dolgoprudnyj, Russia; [6]Pirogov Russian National Research Medical University (RNRMU), Moscow, Russia*

TP 355 **ProteomeGenerator: Integrative Proteomics and Transcriptomics for Non-Canonical Proteome Discovery**; Paolo Cifani[1]; Avantika Dhabaria[2]; Akihide Yoshimi[3]; Omar I. Abdel-Wahab[3]; John T. Poirier[1, 4]; Alex Kentsis[1, 5]; *[1]Molecular Pharmacology Program, Sloan Kettering Institute, Memorial Sloan Kettering Cancer Center, New York, NY; [2]New York University Langone Medical Center, New York, NY; [3]Human Oncology & Pathogenesis Program, Memorial Sloan Kettering Cancer Center, New York, NY; [4]Department of Medicine, Memorial Sloan Kettering Cancer Center, New York, NY; [5]Department of Pediatrics, Weill Medical College of Cornell University and Memorial Sloan Kettering Cancer Center, New York, NY*

TP 356 **Integrated Data Analysis Pipelines for Meta-Omics**; Sujun Li[1]; Yuzhen Ye[1]; Haixu Tang[1]; *[1]Indiana University, Bloomington, IN*

TP 357 **Proteogenomics of Malignant Melanoma Cell Lines: Searching for Genetically Encoded Point Mutations in LC-MS/MS Data**; Anna Lobas[1]; Alexey L Chernobrovkin[2]; Irina Ilina[3]; Dmitry S Karpov[3, 4]; Mikhail Pyatnitskiy[3]; Elizaveta M Solovyeva[1, 5]; Ksenia G Kuznetsova[3]; Mark I Ivanov[1, 5]; Roman Zubarev[2]; Mikhail V Gorshkov[1, 5]; Sergei A Moshkovskii[3]; *[1]INEPCP RAS, Moscow, Russia; [2]Karolinska Institute, Stockholm , Uppland; [3]Institute of Biomedical Chemistry, Moscow, Russia; [4]Engelhardt Institute of Molecular Biology, Moscow, Russia; [5]Moscow Institute of Physics and Technology (State University), Dolgoprudnyj, Russia*

TP 358 **A Linear Algebraic Approach to Combine Top Down and Bottom Up Data and Accurately Determine Protein Modform Distributions**; Philip Compton[1]; Neil L Kelleher[2]; Jeremy Gunawardena[3]; *[1]Northwestern University, Evanston, IL; [2]Northwestern University, Evanston, IL; [3]Harvard Medical School, Boston, MA*

TP 359 **Automated Visualization of Metabolome, Proteome and Fluxome Data on Garuda – a Connectivity Platform for Biomedical Analytics**; Fumio Matsuda[1]; Yohei Yamada[2]; Samik Ghosh[3]; Takeshi Hase[3]; Syohei Kinoshita[1]; Shunsuke Nishino[1]; Atsumi Tomita[1]; Nikolaos Tsorman[3]; Atsuhiko Toyama[2]; Shigeki Kajihara[2]; Norio Mukai[2]; Yukiko Matsuoka[3]; Hiroshi Shimizu[1]; Eiichiro Fukisaki[1]; Hiroaki Kitano[3]; Junko Iida[2, 4]; *[1]Osaka University, Suita, Japan; [2]Shimadzu Corporation, Kyoto, Japan; [3]The Systems Biology Institute, Tokyo, Japan; [4]Osaka University Shimadzu Analytical Innovation Research Laboratory, Suita, Japan*

TP 360 **Phenome Study on the Tissues of Esophageal Squamous Cell Carcinoma**; Guixue Hou[1]; Shaohang Xu[1]; Bo Wen[1]; Xiaomin Lou[2]; Yan Ren[1]; Jin Zi[1]; Siqi Liu[1]; *[1]BGI-Shenzhen, Shenzhen, China; [2]Beijing Institute of Genomics, Chinese Academy of Sciences, Beijing, China*

TP 361 **A Sparse Latent Regression Approach for Integrative Analysis of glycomic and Glycotranscriptomic Data**; Xuefu Wang[1]; Sujun Li[1]; Shiyue Zhou[2]; Yehia Mechref[2]; Haixu Tang[3]; *[1]School of Informatics and Computing, Indiana University, Bloomington, IN - Indiana; [2]Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX; [3]Indiana University, Bloomington, IN*

TP 362 **Multi-Omic Informatics in the Cloud: Galaxy-P Takes a**

Ride on Jetstream; Tim Griffin[1]; Matthew C. Chambers[2]; James E Johnson[1, 3]; Thomas Mcgowan[1, 3]; Thomas Doak[4]; Jeremy Fischer[4]; Praveen Kumar[1]; Pratik Jagtap[1]; *[1]University of Minnesota, Minneapolis, MN; [2]Vanderbilt University, Nashville, TN; [3]Minnesota Supercomputer Institute, Minneapolis, MN; [4]Indiana University Bloomington, Bloomington, IN*

TP 363 **Blood Metabolomics and Transcriptomics Define Metabolic Axes of Human Immune Response to Herpes Zoster Vaccine**; Shuzhao Li[1]; Dean P Jones[1]; Bali Pulendran[1]; *[1]Emory University, Atlanta, Georgia*

TP 364 **A Galaxy-Based, Multi-Staged, Two-Step Searching Pipeline for Improved Peptide Identification in Next Generation Proteomic Studies**; Praveen Kumar[1]; James Johnson[2]; Thomas Mcgowan[2]; Candace R. Guerrero[1]; Pratik Jagtap[1]; Tim Griffin[1]; *[1]University of Minnesota, Minneapolis, MN; [2]Minnesota Supercomputer Institute, Minneapolis, MN*

TP 365 **Enhancing the Multi-omics Visualization Platform (MVP) Plug-in for Galaxy-based Applications**; Thomas Mcgowan[1, 2]; James Johnson[1, 2]; Pratik Jagtap[1]; Praveen Kumar[1]; Getiria Onsongo[1, 2]; Candace R. Guerrero[1]; Tim Griffin[1, 3]; *[1]University of Minnesota, Minneapolis, MN; [2]Minnesota Supercomputer Institute, Minneapolis, MN; [3]Center for Mass Spectrometry and Proteomics, St. Paul, MN*

TP 366 **Transcriptome and Proteome Co-Analysis of High-Fat Diet Induced Hepatic Changes**; Devin Lee Drew[1]; Prasanna Rajagopal[2]; Michelle Puchowicz[3]; Daniela M Schlatzer[3]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Bengaluru, India; [3]Case Western Reserve University School of Medicine, Cleveland, OH*

TP 367 **Proteogenomic Analysis of 31 Human Tissues**; Thomas Wieland[1]; Dongxue Wang[2]; Björn Hallström[3]; Li-Hua Li[2]; Anna Asplund[4]; Mathias Wilhelm[2]; Frederik Ponten[4]; Mathias Uhlen[3]; Hannes Hahne[1]; Bernhard Kuster[5]; *[1]OmicScouts GmbH, Freising, Germany; [2]Technical University of Munich, Freising, Germany; [3]KTH Royal Institute of Technology, Stockholm, Sweden; [4]Uppsala University, Uppsala, Sweden; [5]Technical University Munich, Freising, Germany*

TP 368 **Examining Codon Usage as a Potential Marker of Extracellular Proteins in Microbes**; Alexander Cope[1, 2]; Michael Gilchrist[1]; Robert L Hettich[2]; *[1]University of Tennessee, Knoxville, TN; [2]Oak Ridge National Laboratory, Oak Ridge , TN*

TP 369 **MS-Helios: A Circos Wrapper to Visualize Multi-Omic Datasets**; Harald Marx[1]; Joshua J Coon[1]; *[1]University of Wisconsin-Madison, Madison, WI*

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TP 370 **Multi-Q 2: Automated and Robust Isobaric Labeling Quantitation Analysis with Enhanced Graphical Visualization of Protein Ratio Clustering**; Ching-Tai Chen[1]; Cheng-Wei Cheng[1]; Wei-Jhe Hsu[2]; Hui-Yin Chang[1]; Chu-Ling Ko[3]; T. Mamie Lih[1, 4]; Yi-Ju Chen[4]; Yu-Ju Chen[4]; Wen-Lian Hsu[1]; Ting-Yi Sung[1]; *[1]Institute of Information Science, Academia Sinica, Taipei, Taiwan; [2]Department of Electrical & Computer Engineering, Texas A&M University, College Station, TX; [3]Department of Computer Science, National Chiao Tung University, Hsin Chu, Taiwan; [4]Institute of Chemistry, Academia Sinica, Taipei City, Taiwan*

TP 371 **Automated Identification of Intact N-Linked Glycoproteins with Multiple Protein Search Engines**; Cheng-Wei Cheng[1, 2]; Wen-Lian Hsu[3]; Ting-Yi Sung[3]; *[1]Bioinformatics Program, Taiwan International Graduate Program, Institute of Information Science, Academia Sinica, Taipei, Taiwan; [2]Institute of Biomedical Informatics, National Yang-Ming University, Taipei, Taiwan; [3]Institute of Information Science, Academia Sinica, Taipei, Taiwan*

TP 372 **An Enhanced High-Throughput Quantitation Pipeline to Facilitate Transformative Top-Down Proteomics in the National Resource for Translational and Developmental Proteomics**; Ryan T. Fellers[1]; Richard D. LeDuc[1]; Bryan P. Early[1]; Joseph B. Greer[1]; Alexandra J. Van Nispen[1]; Paul M. Thomas[1]; Neil L. Kelleher[1]; *[1]Northwestern University, Evanston, IL*

TP 373 **PyGrouper: A Gene-Level Inference and Quantification Algorithm for Bottom-Up Proteomics Data**; Alexander B. Saltzman[1]; Mei Leng[1]; Anna Malovannaya[1]; *[1]Baylor College of Medicine, Houston, TX*

TP 374 **Flexible Learning Infrastructure for Proteomics**; Christopher Wilkins[1]; Justice DR Sefas[1]; Aivett Bilbao Pena[1]; Richard D Smith[1]; Ljiljana Pasa-Tolic[1]; Samuel H Payne[1]; Jared B Shaw[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

TP 375 **Building Peptide Spectra Library by Spectral Clustering Using Graphics Processing Units (GPUs)**; Paul TO[1]; Henry LAM[1]; *[1]Division of Biomedical Engineering and Department of Chemical and Biomolecular Engineering, Hong Kong University of Science and Technology, Hong Kong, Hong Kong*

TP 376 **Enhanced Ion Charging Effect of m-Nitro Benzyl Alcohol (m-NBA) on Protein and Peptides Characterization**; Dipankar Malakar[1]; faraz rashid[1]; Manoj Pillai[1]; *[1]ABSCIEX, Gurgaon, Haryana*

TP 377 **Automated Workflow for Host Cell Protein Monitoring by Mass Spectrometry: from Raw Data to Final Report**; Stefano Gotta; *Genedata AG, Basel, Switzerland*

TP 378 **Application of Novel SILAC Analysis Software Proteolabels for Large-Scale Meta-Analysis of Phospho-Proteomes**; Andrew Collins[1, 2]; Antony McCabe[1, 2]; Augustine Amakiri[1]; Ian Morns[3]; Robert Tonge[4]; Johannes P.C. Vissers[4]; Andrew R Jones[1, 2]; *[1]University of Liverpool, Liverpool, UK; [2]Omic Analytics, Liverpool, UK; [3]Waters Corporation, Newcastle upon Tyne, UK; [4]Waters Corporation, Wilmslow, UK*

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TP 379 **Plasma Pyrolysis Mass Spectrometry for the Diagnosis of Leishmaniasis**; Amanda Kretsch[1]; Guido F. Verbeck[1]; *[1]University of North Texas, Denton, TX*

TP 380 **Automatic Construction of t-SRM Methods from Unscheduled SRM Data Raw Files Using the Xcalibur Workbench**; Qingyu Song[1]; Mike Senko[1]; Derek Bailey[1]; Balaram Barange[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

TP 381 **Resonance Effects in a Linear Ion Trap Driven by Rectangular RF Waveforms and AC Signals Applied in Dipolar Mode**; Alexander Lekkas[1]; Andreas Bozatzidis[1]; Dimitris Papanastasiou[2]; *[1]Fasmatech Science & Technology, Athens, Greece; [2]Fasmatech, Athens, Attiki*

TP 382 **A RF Transfer Interface Operable over an Extended Pressure Range for Gating High Mass Ions into an oTOF Mass Spectrometer**; Alexander Lekkas[1]; Dimitris Papanastasiou[2]; Diamantis Kounadis[1]; Emmanuel Raptakis[1]; Gerard van der Laan[3]; Jan Commandeur[3]; *[1]Fasmatech Science & Technology, Athens, Greece; [2]Fasmatech, Athens, Attiki; [3]MS VISION, Almere, Netherlands*

TP 383 **Energy resolved Mass Spectrometry (ER-MS) in UPLC Timescales Using an Orthogonal Acceleration Quadrupole ToF with Novel Fast Acquisition Architecture**; Martin Green[1]; Jason wildgoose[1]; Keith Richardson[1]; Williams Jonathan[1]; Martin Palmer[1]; *[1]Waters Corporation, Wilmslow, UK*

TP 384 **AcroMass MS Processor: a Flexible Data System in Ion Trap Mass Spectrometry for Intact Protein Analysis**; Szu-Wei Chou[1]; Shih-Chieh Yang[1]; Yao-Hsin Tseng[1]; Yi-Kun Lee[1]; Liang-Chun Fan[1]; Chun-Yen Cheng[1]; *[1]AcroMass technologies, Inc., Taipei*

TP 385 **Design and Performance of a Second Generation Cyclic Ion Mobility-Enabled Q-ToF**; Kevin Giles[1]; Jakub Ujma[1]; Jason Wildgoose[1]; Martin R. Green[1]; Keith Richardson[1]; David Langridge[1]; Nick Tomczyk[1]; *[1]Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK*

TP 386 **A Flexible, Cheap, Easy to Construct, and Effective Heater for Small Diameter Polymeric Tubing**; Ryan T. Hilger[1]; James R. Zimmerman[1]; *[1]Jonathan Amy Facility for Chemical Instrumentation, Purdue University, West Lafayette, Indiana*

TP 387 **Application of High Speed TSQ MS with a Prototype RF/DC Rod Driver to Pesticide Analysis**; Harald Oser[1]; Hans Schweingruber[1]; Michael Ugarov[1]; QINGYU SONG[2]; Michael Konicek[2]; Claudia Martins[1]; Neloni Wijeratne[2]; *[1]Thermo Fisher Scientific, San Jose, California; [2]Thermo Fisher Scientific, San Jose, CA*

TP 388 **Realistic Ion Inputs and their Corresponding Instantaneous Current Demands**; Russell Jurek; *ETP Ion Detect, Clyde, NSW*

TP 389 **New Innovations Implemented on the Q Exactive HF Mass Spectrometer**; Tabiwang N. Arrey[1]; Eugen Damoc[1]; Erik Couzijn[1]; Jens Grote[1]; Oliver Lange[1]; Christian Thoeing[1]; Kerstin Strupat[1]; Catherina Crone[1]; Anastassios Giannakopulos[1]; Thomas Moehring[1]; Alexander Harder[1]; *[1]Thermo Fisher Scientific, Bremen, Germany*

TP 390 **Fully Automated Platform for Determination of Benzodiazepines in Serum**; Davide Vecchietti[1]; Claudio Ghilardi[1]; Katharina Kern[2]; Stéphane Moreau[3]; Isabel Cabruja[1]; *[1]Shimadzu Italy, Milan, Italy; [2]Recipe Chemicals + Instruments GmbH, Munich, Germany; [3]Shimadzu Europe GmbH, Duisburg, Germany*

TP 391 **A High Performance OA-ToF Mass Spectrometer for Accurate Mass Measurement of Mobility Separated Ions**; Jason Wildgoose[1]; Martin R. Green[1]; Jakub Ujma[1]; Kevin Giles[1]; *[1]Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK*

TP 392 **Run, MS, Run! Increasing System Robustness with Ion Control**; Brent Lefebvre[1]; Yang Kang[1]; Mauro Aiello[1]; Bradley B Schneider[1]; J.C. Yves Leblanc[1]; *[1]SCIEX, Concord, ON, ON*

TP 393 **Cluster Analysis of Small Organic Molecules by Means of a LTP-Twin-Trap Mass Spectrometer**; Björn Raupers[1]; Claus Köster[2]; Tassilo Muskat[1]; Jürgen Grotemeyer[1]; *[1]Inst. f. Phys. Chem der CAU zu Kiel, Kiel; [2]Bruker Daltonics, Bremen, Germany*

TP 394 **ECD in an RF-Free Electromagnetostatic hv-ExD Cell on a High Resolution/High Throughput Q-Exactive Orbitrap Mass Spectrometer**; Kyle L. Fort[1]; Albert J. R. Heck[1]; Valery G. Voinov[2, 3]; Yury Vasil'ev[2, 3]; Joseph S. Beckman[3]; *[1]Utrecht University, Utrecht; [2]e-MSion, Corvallis, OR; [3]Linus Pauling Institute, Oregon State University, Corvallis, OR*

TP 395 **Ice Formation on Nanoparticles in a Molecular Flow Linear Quadrupole Ion Trap**; Denis Duft[1]; Mario Nachbar[1, 2]; Thomas Dresch[2]; Thomas Leisner[1, 2]; *[1]Institute for Meteorology and Climate Research – Atmospheric Aerosol Research, Karlsruhe Institute of Technology, Karlsruhe, Germany; [2]Institute of Environmental Physics, Ruprecht-Karls-University Heidelberg, Heidelberg, Germany*

TP 396 **RF Trap with Paracell Geometry**; Ekaterina Zhdanova[1]; Vasiliy Eliferov[1]; Igor Popov[1]; Eugene (Evgeny) Nikolaev[1, 2, 3]; *[1]Moscow Institute of Physics and Technology (State University), Dolgoprudnyj, Russia; [2]Skolkovo institute of science and technology, Skolkovo, Russia; [3]Institute of energy problems of chemical physics Russian Academy of Sciences, Moscow, Russia*

TP 397 **Implementation of 213 nm Ultra Violet Photo Dissociation (UVPD) on a Modified Orbitrap Fusion Lumos**; Christopher Mullen[1]; Chad R Weisbrod[2]; Eugene Zhuk[1]; Romain Huguet[1]; Jae C Schwartz[3]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; [3]Thermo Fisher Scientific, San Jose, California*

TP 398 **A Comparative Study of Commercial Electrospray Ionization Sources for Qualitative and Quantitative Proteomic Studies**; Melissa R. Pergande[1]; R.A.C. Rathnayake[1]; Carol Haney-Ball[2]; Vadiraja Bhat[3]; Stephanie M. Cologna[1]; *[1]University of Illinois at Chicago, Chicago, IL; [2]Agilent Technologies Inc., Santa Clara, California; [3]Agilent Technologies, Inc., Wilmington, DE*

TP 399 **Improving MS Performance by Improving High Voltage Power Quality**; James Morrison[1]; Gary Byfield[2]; *[1]Brave-Blue, Manlius, NY; [2]Advanced Energy Industries, Inc., Fort Collins, Colorado*

TP 400 **Determination of the Analytical Figures of Merit for the Qsight Triple Quadrupole**; Joshua Wilhide[1]; Ian W Shaffer[1]; William R LaCourse[1]; *[1]University of Maryland Baltimore County, Baltimore, MD*

TP 401 **Measurement of Effective Radial Geometry of Non-Hyperbolic Linear Ion Trap**; Chuan-Fan Ding; *Fudan University, Shanghai, China*

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TP 402 **Exploring the Benefits and Unique Applications of Cold EI for LC-MS**; Svetlana Tsizin[1]; Tal Alon[1]; Alexander B. Fialkov[1]; Aviv Amirav[1]; *[1]Tel Aviv University, Tel Aviv, Israel*

TP 403 **CHARON PTR-ToF-MS: a New Method for Real-Time Measurement and Molecular-Level Characterization of Submicron Particulate Organic Matter**; Philipp Eichler[1]; Markus Mueller[1, 2]; Andreas Klinger[2]; Armin Wisthaler[1, 3]; Alfons Jordan[2]; *[1]Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Innsbruck, Austria; [2]IONICON Analytik GmbH., Innsbruck, Austria; [3]Department of Chemistry, University of Oslo, Oslo, Norway*

TP 404 **Scent Transmission over the Internet Using Mass Spectrometry**; Fred Paul Mark Jjunju[1]; Giannoukos Stamatios[1]; DANIEL McGuiness[1]; Alan Marshall[1]; Valerio Selis[1]; Jeremy Smith[1]; Simon Maher[1]; Stephen Taylor[1]; *[1]Department of Electrical Engineering and Electronics University Of Liverpool, Liverpool, UK*

TP 405 **Pyrolysis -Vacuum Assisted Plasma Ionization Ion Mobility-Mass Spectrometry for Insoluble Polymer Analysis**; Stephen Zambrzycki[1]; Matthew C Bernier[2]; James Bradshaw[3]; Facundo M Fernandez[4]; *[1]Georgia Institute of Technology, Atlanta, Georgia; [2]Georgia Institute of Technology, Atlanta, GA; [3]Y-12 National Security Complex, Oak Ridge, Tennessee; [4]Georgia Institute of Technology, Atlanta, GA*

TP 406 **Radio Frequency Powered Liquid Sampling-Atmospheric Pressure Glow Discharge (LS-APGD) Ionization Source for Atomic Mass Spectrometry**; Tyler Williams[1]; Kenneth Marcus[1]; *[1]Clemson University, Clemson, SC*

TP 407 **Desorption Ionization Using Through Hole Alumina Membrane (DIUTHAME)**; Yasuhide Naito[1]; Takayuki Ohmura[2]; Masahiro Kotani[2]; *[1]GPI, Hamamatsu, Japan; [2]Hamamatsu Photonics K.K., Iwata, Japan*

TP 408 **Development of a New Atmospheric Pressure Plasmaspray Ionization and Its Comparison with Electrospray Ionization**; Ping Cheng; *School of Environmental and Chemical Engineering, Shanghai University, Shanghai, Shanghai*

TP 409 **Numerical Simulation of Ion Transport in a Nano-Electrospray Ion Source**; Wei Wang[1, 2]; Steve Bajic[1]; Benzi John[2]; David Emerson[2]; *[1]Waters Corporation, Wilmslow, UK; [2]STFC Daresbury Laboratory, Warrington, UK*

TP 410 **Rapid Analysis of Liquid Food Products and Beverages Using Ultrasonic Rapid Evaporative Ionisation Mass Spectrometry**; Daniel Simon[1]; Tamas Karancsi[1]; Steven Derek Pringle[2]; Zoltan Takats[3]; *[1]Waters Research Center,*

Budapest; [2]Waters Wilmslow UK, Wilmslow, Cheshire; [3]Imperial College, London, UK

TP 411 **Improving the Sensitivity of ESI-MS by Efficient Ion Transmission and Desolvation**; Chinthaka A. Seneviratne[1]; Milad Nazari[1]; Elizabeth S. Hecht[1]; Jung Lee[2]; Peter Kottke[2]; Matthew Torres[3]; Andrei G. Fedorov[2]; David C. Muddiman[1]; *[1]W.M. Keck FTMS Laboratory for Human Health Research, Dept. of Chemistry, North Carolina State University, Raleigh, NC; [2]The George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA; [3]School of Biological Sciences, Georgia Institute of Technology, Atlanta, GA*

TP 412 **Charge Reduction and Novel Fragmentation of mAbs with an ESI/Impactor API Source**; Steve Bajic[1]; Jeff Brown[1]; *[1]Waters Corporation, Wilmslow, UK*

TP 413 **Spray Mechanism in Contained-electrospray Ionization Investigated Using On-line Protein Modification**; Colbert Miller[1]; Abraham K. Badu-Tawiah[1]; *[1]Ohio State University, Columbus, OH*

TP 414 **Analysis in Real Time Using Mass Spectrometry Coupled with Plasmas**; Joel Lemaire[1]; Michel Heninger[1]; Essyllt Louarn[1]; Helene Mestdagh[1]; Gérard Bauville[2]; Nicole Blin Simiand[2]; Blandine Bournonville[2]; Michel Fleury[2]; Kristaq Gazeli[2]; Stephane Pasquiers[2]; Sebastien Thomas[1, 2]; Joao Santos Sousa[2]; Elsa Bauchard[3]; Julien Leprovost[3]; *[1]LCP, UMR8000, CNRS-Université Paris Sud, Université Paris Saclay, Orsay, France; [2]LPGP, UMR8578, CNRS-Université Paris Sud, Université Paris Saclay, Orsay, France, Orsay, France; [3]AlyXan, Juvisy sur Orge, France*

TP 415 **Secondary Ion Mass Spectrometry with Individual Projectiles: A Complete Mass Spectrum from a Single Impact?**; Michael J. Eller[1]; Anita Vinjamuri[1]; Gabriel D. Shuffield[1]; Bryan Tomlin[1]; Emile A. Schweikert[1]; *[1]Texas A&M University, College Station, TX*

TP 416 **Improving Spray Stability in Negative Mode Nano-ESI with a Novel Coaxial Sheath Spray Device**; Samuel Wein[1]; Benjamin A. Garcia[2]; *[1]University of Pennsylvania, Philadelphia, Pa; [2]University of Pennsylvania, Philadelphia, PA*

TP 417 **DRy Ion Localization and Locomotion (DRILL) MS Interface for Sensitivity Enhancement *via* Inertial Sorting**; Jung Lee[1]; Peter A. Kottke[2]; Elizabeth S. Hecht[3]; Chinthaka A. Seneviratne[3]; David C. Muddiman[3]; Alex P. Jonke[1]; Matthew P. Torres[2]; Andrei G. Fedorov[2]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]Georgia Institute of Technology, Atlanta, GA; [3]North Carolina State University, Raleigh, NC*

TP 418 **Characterization of Labile Highly Sulfated Cyclodextrins (HSCD) by Cold-Spray Ionization (CSI) Mass Spectrometry**; Daniel Ortiz[1]; Samuel Jones[1]; Francesco Stellacci[1]; Laure Menin[1]; *[1]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*

TP 419 **Ultra High Resolution Atmospheric Pressure Chemical Ionization Evolved Gas Analysis - Gas Chromatography and Thermal Analysis Applied for Petroleum Analysis**; Christopher Paul Rüger[1]; Theo Schwemer[1, 2]; Anika Neumann[1]; Martin Sklorz[1]; Uwe Kaefer[3, 4]; Thomas Groeger[3]; Ralf Zimmermann[1, 2, 5]; *[1]Joint Mass Spectrometry Centre / Chair of Analytical Chemistry, University of Rostock, Rostock, Germany; [2]HICE – Helmholtz Virtual Institute of Complex Molecular Systems in Environmental Health – Aerosols and Health, www.hice-vi.eu, Neuherberg, Germany; [3]Joint Mass Spectrometry Centre, Comprehensive Molecular Analytics, Helmholtz Zentrum München, München, Germany; [4]ASG Analytik Service-Gesellschaft mbH, Neusäss, Germany; [5]Joint Mass Spectrometry Centre / Cooperation Group Comprehensive Molecular Analytics, Helmholtz Zentrum München, Neuherberg, Germany*

TP 420 **Development and Characterization of a New Extractive Electrospray Ionization (EESI) Source for Online Particle Analysis**; Felipe Lopez-Hilfiker[1, 2]; Sonja Klee[1]; Veronika Pospisilova[2]; Manuel Hutterli[1]; Jay Slowik[2]; Andre Prevot[2]; Urs Baltensperger[2]; *[1]TOFWERK, Thun, Switzerland; [2]Paul Scherrer Institute (PSI), Villigen, Switzerland*

TP 421 **Matrix-Free Laser Desorption/Ionization Using Microstructured Anti-Reflection Metal Surfaces**; Jing Yang[1]; Xiaoxiao Ma[1]; Zishuai Li[1]; Jia Jia[2]; Peixun Fan[3]; Minlin Zhong[3]; Zheng Ouyang[1, 4]; *[1]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China; [2]Department of Chemistry, Tsinghua University, Beijing, China; [3]School of Materials Science and Engineering, Tsinghua University, Beijing, China; [4]Weldon School of Biomedical Engineering, Purdue University, West Lafayette, IN*

TP 422 **H2-Plasma for the Generation of Protonation Reagents with a Standard APPI Power Supply**; Hendrik Kersten[1]; Tobias Kutsch[1]; Kai Kroll[1]; Kirsten Haberer[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal*

TP 423 **A New Atmospheric Pressure Ionization Source Using a High Voltage Target Compared to Electrospray Ionization**; Arnaud Lubin[1]; Steve Bajic[2]; Deirdre Cabooter[3]; Patrick Augustijns[3]; Filip Cuyckens[1]; *[1]Janssen R&D, Beerse, Belgium; [2]Waters Corporation, Wilmslow, UK; [3]Department of Pharmaceutical and Pharmacological Sciences, Leuven, Belgium*

TP 424 **Evaluation of a Kinetically Controlled Chemical Ionization Setup**; Kai Kroll[1]; Duygu Erdogdu[1]; Tobias Kutsch[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]Bergische Universität Wuppertal, Wuppertal, NRW*

TP 425 **Improvement of µpCI for Proton Transfer Reactions: a Chambered Ion Source Design for Suppression of Water-Cluster**; Nele Hartmann[1]; David Mueller[1]; Robin Hillen[1]; Yessica Brachthäuser[1]; Klaus J. Brockmann[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]Bergische Universität Wuppertal, Wuppertal, NRW*

TP 426 **nESI-MS Measurement of Protein Melting Temperature Using *theta* Tip Electroosmosis Induced Joule Heating Effect**; Feifei Zhao[1]; Jiexun Bu[2]; Sarah M Matt[2]; Owen G. Rehrauer[3]; Dor Ben-Amotz[2]; Scott A McLuckey[2]; *[1]Purdue University, West Lafayette, IN; [2]Purdue University, West Lafayette, IN; [3]Vertex Pharmaceuticals, Boston, MA*

TP 427 **Adjustable In-Source Fragmentation of Metabolites and Lipids in Laser Desorption Ionization from Silicon Nanopost Arrays**; Andrew Korte[1]; Akos Vertes[2]; *[1]George Washington University, Washington, DC; [2]George Washington University, Washington, DC*

TP 428 **Atmospheric Pressure Temperature Ramped Thermal Desorption/Ionization – Atomic Force Microscope/Mass Spectrometry System for Spatially Resolved Surface Analysis**; Vilmos Kertesz[1]; William D. Hoffmann[1]; Gary J. Van Berkel[1]; *[1]Oak Ridge National Laboratory, Oak Ridge , TN*

TP 429 **Pulsed Valve Inlet Ionization**; Bijay Banstola[1]; Md Amir Hossen[1]; Fabrizio Donnarumma[1]; Kermit K. Murray[1]; *[1]Louisiana State University, Baton Rouge, LA*

TP 430 **Development of an Adaptable, High Sensitivity, Automation for Inlet Ionization**; Milan Pophristic[1]; Sean Rayna[2]; Kevin Rackers[2]; Anil Meher[1, 3]; I-Chung Lu[3]; Ana Djuric[4]; Sarah Trimpin[1, 3]; Charles McEwen[1]; *[1]MSTM, LLC.,, Newark, DE; [2]Automation Techniques, Inc, Greensboro, NC; [3]Department of Chemistry, Wayne State University, Detroit, MI; [4]Engineering Technology, Wayne State University, Detroit, MI*

TP 431 **Electrode-Less Secondary Electrospray Ionization (SESI) for Breath Analysis: Improving the Limits of Detection for Low Volatility Species**; Guillermo Vidal-de-Miguel[1]; Miriam Macia[1]; Pablo Martinez-Lozano Sinues[2];

[1]Fossil Ion Technology, Madrid, Spain; [2]ETH Zurich, Department of Chemistry and Applied Biosciences, Zurich, Switzerland

TP 432 **Comparison of Electrospray and Impactor Ionization for Pharmaceutical Compounds**; Kerri M Smith[1]; Yun Alelyunas[1]; Giorgis Isaac[1]; Joe LaPointe[2]; Nigel Ewing[1]; Mark D Wrona[1]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Beverly, MA*

TP 433 **Spark Discharge Ablation and Ionization of Metalliferous Aerosol Particles**; Thorsten Benter[1]; Joshua Rieger[1]; Steffen Bräkling[1]; Hendrik Kersten[1]; *[1]University of Wuppertal, Wuppertal, Germany*

TP 434 **100% Input Efficient ESI UPLC MS Sample Introduction and MALDI, SIMS, LDI Sample Placement *via* an Inductive Approach. Universal ?**; Drew Sauter[1]; Andrew D. Sauter[1]; Patrick A. Limbach[2]; Robert Ross[2]; Manasses Jora[2]; *[1]Nanoliter, LLC, Henderson , NV; [2]University of Cincinnati, Cincinnati, OH*

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TP 435 **Analysis of Perfluorinated Compounds in Water Using Automated Solid Phase Extraction**; Rudolf Addink[1]; Rashid Juma[1]; *[1]Toxic Report, Watertown, MA*

TP 436 **Determination of Artificial Sweeteners in Water Samples by Liquid-Phase Microextractionn Coupled to Liquid Chromatography-Tandem Mass Spectrometry**; Yu-Hsin Lin[1]; Chung-Yu Chen[1]; Maw-Rong Lee[1]; *[1]National Chung-Hsing University, Taichung, Taichung*

TP 437 **Effective Simultaneous Determination of Five Estrogens in Aqueous Samples Using DLLME and LC-MS/MS**; Seung-Woon Myung[1]; Yeon-Joo Moon[1]; Jun Seok Kim[2]; *[1]Kyonggi University, Suwon-si, South Korea; [2]Korea Polytechnics, Seongnam-si, South Korea*

TP 438 **HPLC/MS/MS Quantitation of Dopamine in Rat Plasma Using AAO Extraction and Derivatization**; Rachel Sun[1]; Tim Shoaf[1]; Robert Clegg[1]; Adrian Bott[1]; *[1]BASi, West Lafayette, IN*

TP 439 **iST: a Reproducible Sample Preparation Method for In-Depth Proteome Discovery and Interaction Proteomics**; Fabian Hosp[1]; Garwin Pichler[1]; Nils A. Kulak[1]; Matthias Mann[2]; *[1]PreOmics, Planegg/Martinsried, Bavaria; [2]Max Planck Institute of Biochemistry, Martinsried, Germany*

TP 440 **Measurement of Pesticides in Apple Juice Using LC-MS/MS with Fast and Modified QuEChERS Extraction Method Using Volatile Buffers**; Avinash Dalmia[1]; Reza Javahery[2]; Lisa Cousins[2]; Scott Lapaglia[3]; Wilhad Reuter[3]; Frenny Kaushal[4]; David welkie[3]; *[1]Perkinelmer, Shelton, CT; [2]PerkinElmer, Woodbridge, ON; [3]PerkinElmer, Shelton , CT; [4]PerkinElmer, Bolton, ON*

TP 441 **A Robust Protocol for Detergent-Free Cell Lysis, Protein Enrichment and Modification with a High Tolerance for Harsh Conditions**; Yannik Lewin; *Department of Pharmaceutical Chemistry, Goethe University, Max-von-Laue-Straße 9, D-60438, Frankfurt am Main, Germany*

TP 442 **Fully Automated Online Sample Preparation and LC-MS/MS Analysis of Drugs of Abuse in Oral Fluids**; Joshua F. Emory[1]; Michael Roberts[1]; Manoj Tyagi[2]; Brian Feild[1]; *[1]Shimadzu Scientific Instruments, Columbia, MD; [2]Captiva Lab, LLC, Charlotte, North Carolina*

TP 443 **Assessment of Solvent Polarity upon Drugs of Abuse in Oral Fluids Using Supported Liquid Extraction (SLE) prior to LC/MS Analysis**; Dan Menasco[1]; Jillian Neifeld[1]; Bruce Kempf[1]; Stephanie J Marin[1]; Elena Gairloch[1]; Helen Lodder[2]; Alan Edgington[2]; Adam Senior[2]; Lee Williams[2]; Paul Roberts[2]; Claire Desbrow[2]; Steve Jordan[2]; *[1]Biotage, Charlotte, NC; [2]Biotage GB Limited, Cardiff*

TP 444 **Comparison of Novel β-Glucuronidases for Process Improvement in Urine Toxicology Workflows**; Phillip R. Gibbs[1]; Hannah M. Milano[1]; Matthew D. Kibbons[1]; *[1]Clinical Lab Consulting of Indiana, LLC, Indianapolis, IN - Indiana*

TP 445 **Simultaneous Extraction of Catecholamine and Metanephrines from Urine Prior to UHPLC-MS/MS Analysis**; Alan Edgington[1]; Adam Senior[1]; Lee Williams[1]; Rhys Jones[1]; Helen Lodder[1]; Geoff Davies[1]; Steve Jordan[1]; Claire Desbrow[1]; Paul Roberts[1]; *[1]Biotage GB Limited, Cardiff*

TP 446 **Thermostable Trypsin/Lys-C Facilitates High-Throughput, Automated Proteomics Sample Preparation for Complex Samples**; Carrie Romer[1]; Danielle B. Gutierrez[1]; Jamie L. Allen[1]; Yuan-wei Nei[1]; Melissa A. Farrow[2]; Nikesh Dahal[2]; Jocelyn Simpson[2]; Salisha Hill[1]; Kristie L. Rose[1]; Jeremy L. Norris[1]; Michael Rosenblatt[3]; Eric P. Skaar[2]; D. Borden Lacy[2]; Richard M. Caprioli[1]; *[1]MSRC Vanderbilt University, Nashville, TN; [2]Vanderbilt University Medical Center, Nashville, TN; [3]Promega Corporation, Madison, WI*

TP 447 **Screening and Quantitation of over 200 Pesticides/Antibiotics in Honey Using the eXtreme|FV for Sample Prep and On-Line Extraction UHPLC-MS/MS Analysis**; Sam Ellis; *Thomson Instrument Company, Oceanside, CA*

TP 448 **Electromagnetic Mixer for Highly Efficient, Automated Sample Preparation**; Chang Liu[1]; Don W Arnold[2]; Thomas R. Covey[1]; *[1]SCIEX, Concord, ON; [2]SCIEX, Redwood City, CA*

TP 449 **Method Optimization for the Low Level Detection of Vitamin B7 from Human Serum Using UPLC-MS/MS Analysis**; Lee Williams[1]; Helen Lodder[1]; Rhys Jones[1]; Alan Edgington[1]; Adam Senior[1]; Geoff Davies[1]; Steve Jordan[1]; Claire Desbrow[1]; Paul Roberts[1]; *[1]Biotage GB Limited, Cardiff*

TP 450 **Therapeutic Drug Monitoring of Antiepileptic Drugs in Serum: a Fully Automated Approach**; Davide Vecchietti[1]; Claudio Ghilardi[2]; Stéphane Moreau[3]; Stephan Schröder[4]; Katharina Kern[5]; Isabel Cabruja[2]; *[1]Shimadzu, Milan, Lombardy; [2]Shimadzu Italy, Milan, Italy; [3]Shimadzu Europe GmbH, Duisburg, Germany; [4]Shimadzu Deutschland GmbH, Duisburg, Germany; [5]Recipe Chemicals + Instruments GmbH, Munich, Germany*

TP 451 **Enhanced Lipids Removal from Biological Matrices to Prepare Samples for LC/MS/MS Analysis**; Limian Zhao[1]; Derick Lucas[2]; *[1]Agilent Technologies, Wilmington, DE; [2]Agilent Technologies, Inc., Wilmington, DE*

TP 452 **Online Extraction of Antihypertensive Drugs from Human Serum Samples by LC-MS/MS Analysis**; Carolina Tosin Bueno[1]; Henrique Dipe de Faria[2]; Eduardo Costa Figueiredo[2]; Jose Eduardo Krieger[1]; Eduardo Moacyr Krieger[1]; Alexandre Costa Pereira[1]; Paulo Caleb Junior Lima Santos[1]; *[1]Laboratory of Genetics and Molecular Cardiology, Heart Institute (InCor), University of Sao Paulo, Medical School, Sao Paulo, Brazil; [2]Laboratory of Toxicant and Drug Analysis, University of Alfenas - Unifal-MG, Alfenas, Brazil*

TP 453 **Development of a Simple and Sensitive Derivatization Method for LC/MS/MS Analysis of Epinephrine in high Salt Contained Buffer Solutions**; Bih-Hsiung Hsu[1]; Patrick Lin[1]; *[1]PHARMout Lab, Sunnyvale, CA*

TP 454 **LC/MS/MS Bioanalytical Protocol for Determining the Degree of Non-Specific Binding in Multi-Well Plates**; Liyun Zhang[1]; Jack Henion[1]; *[1]Q2 Solutions, Ithaca, NY*

TP 455 **LC-MS/MS Assay Miniaturization in Support of ABS Microsampling Pharmacokinetics Studies**; Elizabeth A. Mahan[1]; Ken Anderson[2]; Jacqueline Kenny[2]; Rena Zhang[2]; *[1]Merck & Co., West Point, PA; [2]Merck & Co., West Point, PA*

TP 456 **Comparison of Manual and Automated Sample Preparation Techniques for Lipidomics**; Linda Ahonen[1]; Peter Rossing[1]; *[1]Steno Diabetes Center Copenhagen, Gentofte, Denmark*

TP 457 **Sample Preparation Strategies for Urine Panels with 50 of More Drugs and Metabolites Analyzed by LC-MS/MS**; Stephanie J Marin[1]; Dan Menasco[1]; Jillian Neifeld[1]; Elena Gariloch[1]; *[1]Biotage, Charlotte, NC*

TP 458 **Quantitative Analysis of THC and related cannabinoids in Multiple Matrices Using Simplified Solid Phase Extraction with UPLC/MS/MS**; XIN ZHANG[1]; Jonathan Danaceau[2]; Erin Chambers[2]; Kim Haynes[2]; *[1]Waters Corp, Milford, MA; [2]Waters Corporation, Milford, MA*

TP 459 **Improved LC/MS/MS Analysis of Vitamin D Metabolites in Biological Samples Using Enhanced Matrix Removal Sample Preparation** ; Derick Lucas[1]; Limian Zhao[2]; *[1]Agilent Technologies, Wilmington, DE; [2]Agilent Technologies, Inc., Wilmington, DE*

TP 460 **Development of a LC-MS/MS Method for Quantitative Measurement of Drugs in Microscale 3D Bioprinted Human Liver Samples**; Emily Adarayan[1]; Elizabeth A. Mahan[1]; Guangping Bi[1]; Gary Adamson[1]; Rena Zhang[1]; Andreas Baudy[1]; *[1]Merck Reseach Labs, West Point, PA*

TP 461 **Organic Flush Solutions to Remove Sample Matrix Interferences in LC-MS Systems** ; Haibo Wang[1]; Stephen C Roemer[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Fair Lawn, NJ - New Jersey*

TP 462 **Optimized SPE-LC/MS/MS Assay to Support Measurement Released Drug in Nanoparticle Formulation** ; Wei Song[1]; Brian Rago[1]; Yizhong Zhang[1]; Eyoung Shin[1]; Young-Ho Song[1]; Aarif Ahsan[1]; Ravi Visswanathan[1]; Mauricio Leal[1]; Chris Holliman[1]; *[1]Pfizer, Groton, CT*

TP 463 **Drugs of Abuse in Oral Fluids: Automated SPE Extraction and LC/MS/MS Analysis Using a Robotic Autosampler**; Fred Foster [1]; John R. Stuff[1]; Edward A. Pfannkoch[1]; Mark Hayward[2]; *[1]Gerstel, Inc., Linthicum , MD; [2]ITSP Solutions, Hartwell, GA 30643*

TP 464 **Method Development Strategies Using Polymer-Based SPE for the Analysis of Peptides Prior to UPLC-MS/MS Analysis**; Helen Lodder[1]; Lee Williams[1]; Rhys Jones[1]; Adam Senior[1]; Alan Edgington[1]; Geoff Davies[1]; Steve Jordan[1]; Claire Desbrow[1]; Paul Roberts[1]; *[1]Biotage GB Limited, Cardiff, UK*

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TP 465 **Facile Analysis of Sterols by Thiol-Based Photochemical Tagging and Electrospray Ionization – Mass Spectrometry**; Sarju Adhikari[1]; Yu Xia[1]; *[1]Purdue University, West lafayette, Indiana*

TP 466 **Study on Triacylglycerides in Edible Vegetable Oils by Ultra-High Performance Liquid Chromatography Tandem Quadrupole-Time Of Flight Mass Spectrometry**; Jianzhong Li[1]; Yao Xiao[2]; Xin Ma[2]; Qilei Guo[2]; Tao Bo[2]; *[1]Agilent Technologies(China), Beijing, Beijing; [2]Agilent Technologies (China), Beijing, China*

TP 467 **Comprehensive Analysis of N-Acylethanolamine and Monoacylglycerol Species by Shotgun Lipidomics**; Kazuo Kanaya[1]; Miao Wang[1]; Xianlin Han[1]; *[1]Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL*

TP 468 **Effects of Heparin Versus EDTA Anti-Coagulant on Plasma Samples Analyzed Using the LipidyzerTM Platform**; Richard J. Robinson[1]; Philip M. Charpia[1]; Uyenthao T. Nguyen[1]; Anne M. Evans[1]; Luke A.D. Miller[1]; *[1]Metabolon, Inc., Durham, NC*

TP 469 **Evaluation of Hepatic Lipids from Rabbits under Conditions Stimulating Non-Alcoholic Fatty Liver Disease Using Nanoflow UPLC-ESI-MS/MS**; Seul Kee Byeon[1]; Myeong Hee Moon[1]; *[1]Yonsei University, Seoul, South Korea*

TP 470 **Shotgun Lipidomics Reveals Decreases in Myelin Lipid Content in the Central and Peripheral Nervous Systems of db/db Mice**; Chunyan Wang[1]; Palavicini Pablo Juan[1]; Linyuan Chen[1]; Jianing Wang[1]; Xianlin Han[1]; *[1]Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL*

TP 471 **Probing the Electrostatic Interactions between Cationic Antimicrobial Peptides and Kdo2-Lipid A *via* Ultraviolet Photodissociation Mass Spectrometry**; Christopher M Crittenden[1]; Lindsay J Morrison[1]; Lucas D Akin[1]; Bryan W Davies[2, 3]; Jennifer S Brodbelt[1]; *[1]Department of Chemistry, University of Texas at Austin, Austin, TX; [2]Department of Molecular Biosciences, University of Texas at Austin, Austin, TX; [3]Institute of Cellular and Molecular Biology, University of Texas at Austin, Austin, TX*

TP 472 **HCD-Analysis of Human Blood Plasma Lipid Classes *via* Combinatorial Free Fatty-Acid and Solid Phase Extraction of Phospho-, Glycero-, and Sphingolipids**; Tobias M Maile[1]; Eugene Melamud[1]; Bryson Bennett[1]; *[1]Calico LLC, South San Francisco, CA*

TP 473 **Lipid Parameters Associated with Obesity Identified Using a High-Throughput Shotgun Lipidomics Technology**; Christian Klose[1]; Michal A. Surma[1]; Ronny Herzog[1]; Mathias Gerl[1]; Elena Sokol[2]; David Peake[3]; Céline Fernandez[4]; Olle Melander[4, 5]; Kai Simons[1]; *[1]Lipotype GmbH, Dresden, Saxony; [2]Thermo Fisher Scientific-, Hemel Hempstead, UK; [3]Thermo Fisher Scientific, San Jose, CA; [4]Department of Clinical Sciences, Lund University, Malmö, Sweden; [5]Department of Internal Medicine, Malmö, Sweden*

TP 474 **Recent Improvements in TrEnDi: Lipid Scope and Signal Consolidation**; Carlos R. Canez[1]; Gilian T. Thomas[1]; Samuel W.J. Shields[1]; Karl V. Wasslen[1]; Peter J. Pallister[1]; Jeffrey M. Manthorpe[1]; Jeffrey C. Smith[1]; *[1]Carleton University, Ottawa, ON*

TP 475 **Size Fractionation Coupled to Lipid and Protein Measurements to Quantify Lipoprotein Particle Number and Composition in Normal and Dyslipidemic Subjects**; Michael Gardner[1]; Zsuzsanna Kuklenyik[1]; David M Schieltz[1]; Bryan A Parks[1]; Jon Rees[1]; Lisa McWilliams[1]; Christopher Toth[1]; Jeffrey Jones[1]; Michael Andrews[1]; Antony Lehtikoski[1]; John Barr[1]; *[1]Centers for Disease Control and Prevention, Atlanta, GA*

TP 476 **Identification and Quantification of Lecithin Phospholipid in Freeze Dried and Drum Dried Fruit and Vegetable by LC-MS and HPLC-ELSD**; Xiaoyan Xia[1]; Boris V. Nemzer[2, 3]; *[1]FutureCeuticals Inc., Momence, IL; [2]FutureCeuticals Inc., Momence, iL; [3]Department of Food Science and Human Nutrition, University Illinois at Urbana Champaign, Urbana, IL*

TP 477 **Quantitation of Phospholipids Based on Isotope-Labeled Methylation Using nUPLC-ESI-MS/MS**; Jong Cheol Lee[1]; Seul Kee Byeon[1]; Myeong Hee Moon[1]; *[1]Yonsei University, Seoul, South Korea*

TP 478 **Fragmentation Behavior of Neuronal Lipids by HCD-MS/MS**; Tommy Hofmann[1]; Carla Schmidt[1]; *[1]Interdisciplinary research center HALOmem, Martin Luther University Halle-Wittenberg, Halle (Saale), Germany*

TP 479 **Synaptamide Biosynthesis Monitored by Stable Isotope Labeling and High Resolution Mass Spectrometry**; Karl Kevala[1]; Michel Lagarde[2]; Arthur Spector[1]; Hee-Yong Kim[1]; *[1]National Institutes of Health, NIAAA, Rockville, MD; [2]Universite de Lyon, INSA, Villeurbanne, France*

TP 480 **Automated Lipid Profiling of a Plasma Sample Using Ultra-High Resolution Qq-Time-Of-Flight Impact II™ Mass Spectrometer with SimLipid Software**; Ningombam Sanjib Meitei[1]; Himani Gupta[1]; Arun Apte[2]; Aiko Barsch[3]; Anjali Alving[4]; Juan J Aristizabal Henao[5]; Ken D Stark[5]; *[1]PREMIER Biosoft, Indore, India; [2]PREMIER Biosoft, Palo Alto, CA; [3]Bruker Daltonik GmbH, Bremen, Germany; [4]Bruker Daltonic, Billerica, MA; [5]University of Waterloo, Waterloo, Ontario*

TP 481 **Lipidomic Analysis of Urinary Exosomes According to their Sizes by Flow Field-Flow Fracionatation and nUPLC-ESI-MS/MS**; Joon Seon Yang[1]; Myeong Hee Moon[1]; *[1]Yonsei University, Seoul, South Korea*

TP 482 **The Role of Decreased Mitochondria Phospholipid and Impaired Electron Transport Chain for Brain Damage in Cardiac Arrest** ; Jonathan Tam[1]; Angela Hong[2]; Tai Yin[3]; Junhwan Kim[3]; *[1]Hofstra Northwell School of Medicine, Hempstead, NY; [2]Villanova University, Villanova, PA; [3]Feinstein Institute for Medical Research, Manhasset, NY*

TP 483 **Investigating the Pathways of Lipid Biosynthesis in *C. reinhardtii* under Nitrogen Starvation Conditions Using Isotope Labeling and LC-MS**; Carter Lantz[1]; Matthew Brantley[1]; James Chang[1]; Jeremy Sieker[1]; Sung-Joon Kim[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, Texas*

TP 484 **Authentication of Two Different Types of Fish Oils by Qualitative Lipid Profiling Using Semi-Targeted Approach on QTRAP Platforms**; Niladri Sekhar Chatterjee[1]; Akanksha Singh[2]; Vishnu KV[1]; Ajeeshkumar K K[1]; Anandan R[1]; Ashok Kumar[1]; Suseela Mathew[1]; Manoj Pillai[2]; *[1]ICAR-Central Institute of Fisheries Technology, Cochin, India; [2]SCIEX, 121, Udyog Vihar, Phase IV., Gurugram, India*

TP 485 **Identification of Ligands for YF1*7.1, a Novel MHC Class I-Like Molecule**; Gabriel Gugiu[1, 2]; Ronald Goto[3]; Marcia Miller[3]; *[1]City of Hope, Molecular immunology - BRI, Duarte, CA; [2]City of Hope, Shared Resources - BRI, Duarte, CA; [3]City of Hope, Molecular & Cellular Biology - BRI, Duarte, CA*

TP 486 **Enhanced Coverage of Lipid Analysis and Imaging by MALDI-MS *via* a Strategy with an Optimized Mixture of Matrices**; Jianing Wang[1]; Chunyan Wang[1]; Xianlin Han[1]; *[1]Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL*

TP 487 **Comprehensive Global Lipidomics Profiling on LC-MS/MS Timeframe with Quadrupole Orbitrap Mass Spectrometer Detection**; Josef Ruzicka[1]; David A. Peake[2]; *[1]Thermo Fisher Scientific, Somerset, NJ; [2]ThermoFisher, San Jose, CA*

TP 488 **Next Generation Lipid Profiling of Human Red Blood cells Unmasks Hidden Diversity**; Amani M Batarseh[1]; Sarah K Abbott[1]; Ayedh Alqarni[1]; Stephen J Blanksby[2]; Todd W Mitchell[1]; *[1]University of Wollongong, Wollongong, NSW; [2]Queensland University of Technology, Brisbane, Australia*

TP 489 **Lipidomic Responses of Stem Cells to Microfabricated Structures Using MALDI-MS**; Martin R. L. Paine[1]; Nick R. M. Beijer[2]; Jan De Boer[2]; Ron M. A. Heeren[1]; Shane R. Ellis[1]; *[1]M4I Institute - Maastricht University, Maastricht, Netherlands; [2]MERLN Institute, Maastricht, Netherlands*

TP 490 ***in situ* and Plasma Phospholipidome Studies of Rats Following Ischemic Stroke**; Hay-Yan J. Wang[1]; Erh-Hsuan Hsiang[1]; Zhi-Fu Zheng[2]; *[1]National Sun Yat-Sen University, Kaohsiung, Taiwan; [2]Hyper Quantum Technologies, Kaohsiung, Taiwan*

MALDI: SAMPLE PREPARATION
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TP 491 **Physical Vapor Deposition Screening for Nanoparticle Assisted Laser Desorption Ionization Mass Spectrometry Applied to Microbiome Metabolomics**; Rebecca Hansen[1]; Maria Emilia Dueñas[1]; Gargey Yagnik[1]; Young-Jin Lee[1]; *[1]Iowa State University, Ames, IA*

TP 492 **The Molecular Scanner Approach: Applications in Tissue Imaging**; William Andrews[1]; Merlin Bruening[1]; Amanda B. Hummon[1]; *[1]University of Notre Dame, Notre Dame, IN*

TP 493 **Metal Organic Frameworks as a New Class of MALDI Matrices**; Rabih Jabbour[1]; Gregory W. Peterson[2]; Jared B. Decoste[2]; *[1]ECBC, APG, MD; [2]ECBC, US Army, Gunpowder, MD*

TP 494 **Enhancing Ion Abundances of Carbohydrates by Controlling Sample Crystalline Structures in MALDI Mass Spectrometry**; Yu-Meng Ou[1, 2]; Hsun Lee[1]; Yin-Hung Lai[1]; Huan-Tsung Chang[2]; Yi-Sheng Wang[1]; *[1]Genomics Research Center Academia Sinica, Taipei; [2]Department of Chemistry, National Taiwan University, Taipei, Taiwan*

TP 495 **Non-Commerical MALDI Matrices for the Analysis of Acidic Peptides**; Xinyao Jing[1]; Kyle Edwards[1]; John B. Vincent[1]; Angelo James[1]; Yuping Bao[1]; Carolyn J Cassady[1]; *[1]The University of Alabama, Tuscaloosa, AL*

TP 496 **Improved Quantitative Analysis in MALDI-MS Using Freeze Vacuum Drying**; Dongwon Shin[1]; Jihyun Paek[1]; Jeongkwon Kim[1]; *[1]Chungnam National University, Daejeon, Daejeon*

TP 497 **Coffee Ring Effect Enhacement of Biomolecule Signals by MALDI**; Laura J Castellanos-García[1]; Alyssa L. M Marsico[1]; Bradley Duncan[1]; Ryan F. Landis[1]; Gulen Yesilbag Tonga[1]; Vincent M Rotello[1]; Richard W Vachet[1]; *[1]University of Massachusetts-Amherst, Amherst, MA*

TP 498 **Effect of Additive Cation on the Analysis of Sucrose Using MALDI-MS**; Jihyun Paek[1]; Jeongkwon Kim[1]; *[1]Chungnam National University, Daejeon, Daejeon*

TP 499 **New Fixed-Charge Derivatization Agents for Analysis of Carbonyl Compounds by MALDI, SALDI and ESI Mass Spectrometry**; Larisa Kulikova[1]; Valentina Ilyushenkova[1, 2]; Dmitrii Zhilyaev[1, 2]; Roman Borisov[1, 3]; *[1]RUDN University, Moscow, Russia; [2]Topchiev Institute of Petrochemical synthesis, Moscow; [3]Topchiev Institute of Petrochemical synthesis, Moscow*

TP 500 **Combined Solid and Liquid Matrix High Vacuum Sublimation and Evaporation Coating for MALDI Imaging**; Fan Cao[1]; Fabrizio Donnarumma[1]; Md Amir Hossen[1]; Kermit K. Murray[1]; *[1]Louisiana State University, Baton Rouge, LA*

TP 501 **Covalent Linkage of Matrix for Enhanced MALDI-MS**; Jason Williams; *NIEHS, RTP, NC*

TP 502 **Development of a Novel Sample Preparation Approach for Bottom-Up Shotgun Proteomics**; Simona Salivo[1]; Tom K. Abban[1]; Emanuele Barborini[2]; Matthew E. Openshaw[1]; *[1]Shimadzu, Manchester, UK; [2]Tethis SpA, Milan, Italy*

TP 503 **Direct On-Plate Desalting and Enrichment for Improved Low Molecular Weight Marker Detection**; Mohamed Nazim Boutaghou[1]; Sharath Hosali[2]; Jason Sakamoto[2]; Brian Feild[1]; *[1]Shimadzu Scientific Instr., Columbia, MD; [2]NanoMedical Systems, Houston, TX*

METABOLOMICS: UNTARGETED METABOLITE PROFILING II
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TP 504 **Metabolomic Profiling of NGLY1 Deficiency Disease**; Songjie Chen[1]; Guangwen Wang[1]; David Marciano[1]; Michael Snyder[1]; *[1]Stanford University School of Medicine, Stanford, CA*

TP 505 **Application of GC Orbitrap Mass Spectrometry for Untargeted Metabolomics of Pathogenic Microorganisms**; Fausto Pigozzo[1]; Cristian Cojocariu[2]; Paul Silcock[2]; Stefan Weidt[3]; Jeni Haggarty[3]; Karl Burgess[3]; *[1]Thermo Fisher Scientific, Rodano, Milano; [2]Thermo Fisher Scientific-, Runcorn, UK; [3]Glasgow Polyomics, University of Glasgow, Glasgow, UK*

TP 506 **Rapid Threat Analysis –A Workflow to Support Metabolomics Analysis of a Cell's Response to an Unidentified Toxin in 30 Days**; Randi Gant-branum[1]; Stacy D. Sherrod[2]; Simona Gabriela Codreanu[2]; Alexandra C Schrimpe-Rutledge[2]; James M Poland[2]; Jerry Holman[2]; Nicole Muszynski[2]; James C Pino[2]; Carrie E. Romer[2]; Jamie L. Allen[2]; Richard M. Caprioli[2]; John A. McLean[2]; *[1]Vanderbilt University, Nashville, tenn; [2]Vanderbilt University, Nashville, TN*

TP 507 **Global Metabolomic Profiling Identifies Novel Mechanisms of Cuprizone-Mediated Oligodendrocyte Dysfunction**; Alexandra Taraboletti[1]; Tia Walker[2]; Robin Avila[3]; He Huang[1]; Joel Caporoso[4]; Erendra Manandhar[1]; Thomas Leeper[5]; David Modarelli[1]; Satish Medicetty[3]; Leah Shriver[1]; *[1]University of Akron, Akron, OH; [2]Indiana University Northwest, Gary, IN; [3]Renovo Neural, Inc., Cleveland, OH; [4]University of Pittsburgh School of Medicine, Pittsburgh, PA; [5]College of Wooster, Wooster, OH*

TP 508 **Evaluation of the Metabolism of Azo Dyes and its Effects on the *Staphylococcus aureus* Metabolome**; Jinchun Sun [1]; Jinshan Jin[2]; Richard D. Beger[3]; Carl E. Cerniglia[4]; Huizhong Chen[4]; *[1]NCTR / USFDA, Jefferson , AR; [2]Division of Microbiology, Jefferson, AR; [3]Division of System Biology, National Center for Toxicological Research, Jefferson, AR; [4]Division of Microbiology, National Center for Toxicological Research, Jefferson, AR*

TP 509 **Metabolite Fragmentation in Laser Ablation Electrospray Ionization Mass Spectrometry with Ion Mobility Separation**; Ziad Sahab[1]; Sylwia Stopka[1]; Bindesh Shrestha[2]; Hang Li[3]; Wei Yuan[1]; Lida Parvin[1]; Akos Vertes[1]; *[1]George Washington University, Washington, DC; [2]Waters Corporation, Beverly, MA; [3]George Washington University , Washington, DC*

TP 510 **Metabolomic Profiles of Normal Airway Epithelium Cells Upon Exposure to Cigarette Smoking Condensate**; Alexandra C Schrimpe-Rutledge[1, 2]; Xiangming Ji[3, 4]; Simona Gabriela Codreanu[1, 2]; Stacy D. Sherrod[1, 2]; Pierre D Massion[5, 6, 7]; John A. McLean[1, 2, 8, 9]; *[1]Department of Chemistry, Vanderbilt University, Nashville, TN; [2]Center for Innovative Technology, Vanderbilt University, Nashville, TN; [3]Division of Allergy, Pulmonary and Critical Care Medicine, Vanderbilt University School of Medicine, Nashville, TN; [4]Vanderbilt Ingram Comprehensive Cancer Center, Vanderbilt University School of Medicine, Nashville, TN; [5]Division of Allergy, Pulmonary and Critical Care Medicine, Department of Medicine, Cancer Early Detection and Prevention Initiative, Vanderbilt Ingram Cancer Center, Nashville, TN; [6]Department of Cancer Biology, Vanderbilt University Medical Center, Nashville, TN; [7]Veterans Affairs, Tennessee Valley Healthcare System, Nashville, TN; [8]Vanderbilt Institute of Chemical Biology, Vanderbilt University, Nashville, TN; [9]Vanderbilt Institute for Integrative Biosystems Research and Education, Vanderbilt University, Nashville, TN*

TP 511 **A Lipidomics Characterization of Zika-Infected Mosquito Cells**; Carlos Fernando Odir Rodrigues Melo[1]; Diogo Noin de Oliveira[1]; Estela de Oliveira Lima[1]; Tatiane Melina Guerreiro[1]; Cibele Zanardi Esteves[1]; Rodrigo Ramos Catharino[1]; *[1]Innovare Biomarkers Laboratory, Campinas, Brazil*

TP 512 **High throughput Metabolomics Using FTICR-MS to Reveal Rat Exposure States to Pesticides**; Baninia Habchi[1, 2]; Sandra Alves[2]; Delphine Jouan-Rimbaud Bouveresse[1]; Brice Appenzeller[3]; Douglas N. Rutledge[1]; Alain Paris[4]; Estelle Rathahao-Paris[1]; *[1]UMR Ingénierie Procédés Aliments, AgroParisTech, Inra, Université Paris-Saclay, Massy, France; [2]Sorbonne Universités, UPMC Univ Paris 06, CNRS, Institut Parisien de Chimie Moléculaire (IPCM), Paris, France; [3]Human Biomonitoring Research Unit, Luxembourg Institute of Health (LIH), Rue Henri Koch 29, Esch-sur-Alzette, Luxembourg; [4]Sorbonne Universités, Muséum national d'Histoire naturelle, CNRS, UMR7245 MCAM, Paris, France*

TP 513 **LC/ MS-Based Lipidomic Profiling in Heart Tissue of Mice with Diet-Induced Atherosclerosis**; Sunhee Jung[1]; Miso Nam[1]; Do Hyun Ryu[2]; Geum-Sook Hwang[1]; *[1]Korea Basic Science Institute, Seoul, South Korea; [2]Sungkyunkwan University, Suwon, South Korea*

TP 514 **Single-Probe MS Analysis of Extracellular Metabolites in Live *in vitro* Tumors**; Mei Sun[1]; Ning Pan[1]; Zhibo Yang[2]; *[1]University of Oklahoma, Norman, OK; [2]University of Oklahoma, Norman, OK*

TP 515 **Profiling Strategies for Discovery of Acylated Specialized Metabolites**; Steven M. Hurney[1]; Gaurav D. Moghe[1]; Robert L. Last[1]; A. Daniel Jones[1]; *[1]Michigan State University, East Lansing, MI*

TP 516 **High Throughput Metabolomics by Ion Mobility Mass Spectrometry**; Sandra Alves[1]; Alain Paris[2]; Guillaume Van der Rest[3]; Estelle Rathahao-Paris[4]; *[1]Sorbonne Universités, UPMC Univ Paris 06, CNRS, Institut Parisien de Chimie Moléculaire (IPCM), Paris, France; [2]Sorbonne Universités, Muséum national d'Histoire naturelle, CNRS, UMR7245 MCAM, Paris, France; [3]Université Paris Sud, Laboratoire de Chimie Physique, Orsay, France; [4]UMR Ingénierie Procédés Aliments, AgroParisTech, Inra, Université Paris-Saclay, Massy, France*

TP 517 **Development of a Serum Metabolome Database Using Isotope Labeling and High-resolution LC-MS**; Wei Han[1]; Minglei Zhu[1]; Ngoc Tran Tran[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB*

TP 518 **Mass Spectrometric Investigation of the Human Gut Microbiota's Response to Infection as a Source for Novel Antibiotics**; Caitlin Keller[1]; Jennifer Bratburd[1]; Cameron Currie[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

TP 519 **A Metabolomics Approach to Dissecting γ–Aminobutyrate Metabolism and its Link to Virulence and Reproduction in the Wheat Pathogen *Parastagonospora nodorum***; Hayley Abbiss[1, 2, 3]; Oliver Mead[4]; Susan Breen[4]; Joel P A Gummer[1, 2]; Stacey N Reinke[1, 2]; Robert D Trengove[1, 2]; Peter S Solomon[4]; *[1]Separation Science and Metabolomics Laboratory, Murdoch University, Perth, Australia; [2]Murdoch University, Perth, Western Australia; [3]SpectralWorks, Runcorn, UK; [4]Research School of Biology, The Australian National University, Canberra, Australia*

TP 520 **Modifying Skin Metabolome and Microbiome with Personal Care Products**; Amina Bouslimani[1]; Ricardo Silva[1]; Amnon Amir[2]; Tomasz Kosciolek[2]; Stefan Janssen[2]; Kathleen Dorrestein[1]; Gregory Humphrey[2]; James Gaffney[2]; Tara Schwartz[2]; Karenina Sanders[2]; Alexey V Melnik[1]; Chris Callewaert[2]; Tal Luzzatto-Knaan[1]; Rob Knight[2, 3, 4]; Pieter C. Dorrestein[1, 2, 4, 5]; *[1]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; [2]Department of Pediatrics, University of California San Diego, La Jolla, CA; [3]Department of Computer Science and Engineering, University of California San Diego, La Jolla, CA; [4]Center for Microbiome Innovation, University of California San Diego, La Jolla, CA; [5]Department of Pharmacology, University of California San Diego, La Jolla, CA*

TP 521 **Dietary Effects on the Human Urine Metabolome: A Case Study Involving Cow Milk Consumption**; Dorothea Mung[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB*

TP 522 **Discovery of Biomarkers of Brain Tumor Metastasis in a Medulloblastoma Mouse Model**; Danning Huang[1]; Martin R. L. Paine[1]; Jingbo Liu[2]; David A. Gaul[1]; Tobey J. MacDonald[2]; Facundo M. Fernández[1]; *[1]School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA; [2]Aflac Cancer and Blood Disorders Center, Department of Pediatrics, Emory University School of Medicine, Atlanta, GA*

TP 523 **Using Non-Targeted High Resolution LC-QTOF Profiling to Characterize Metabolic Responses of *Nicotiana attenuata* during Infection with *Rhizophagus irregularis***; Sven Heiling[1]; Ming Wang[1]; Rayko Halitschke[1]; Emmanuel Gaquerel[2]; Aiko Barsch[3]; Magdalene Reinkensmeier[3]; Ian T Baldwin[1]; *[1]Max Planck Institute for Chemical Ecology, Department for Molecular Ecology, Jena, Germany; [2]Centre*

for Organismal Studies Heidelberg, University of Heidelberg, Heidelberg, Germany; [3]Bruker Daltonics, Bremen, Germany

TP 524 **Profiling of Wine Using Ultra-High Resolution Flow Injection Mass Spectrometric Analysis and 1H-NMR Spectroscopy**; Matthias Witt[1]; Nikolas Kessler[1]; Markus Godejohann[2]; Michael L. Easterling[3]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Bruker BioSpin GmbH, Rheinstetten, Germany; [3]Bruker Daltonic, Billerica, MA*

TP 525 **An Untargeted Metabolomics Approach to Using High Resolution Mass Spectrometry for Identifying Disease Biomarkers**; GINA TAN[1]; Svetlana Rezinciuc[2]; Heather S. Smallwood[2]; Andreas F. Huhmer[3]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]University of Tennessee Health Science Center, Memphis, TN; [3]Thermo Fisher Scientific, San Jose, CA*

TP 526 **A Metabolomics Study on crtEBI Recombinant *Saccharomyces cerevisiae* with UHPLC Tandem Quadrupole-Time of Flight Mass Spectrometry**; Wei Du[1]; TAO BO[1]; *[1]Agilent Technologies, Beijing, China*

TP 527 **Biomarkers for Human Plasma Sample Quality Using an IROA-Labeled Universal Internal Standard**; Casey A. Chamberlain[1]; Chris Beecher[2]; Timothy J. Garrett[1]; *[1]University of Florida, Gainesville, FL; [2]IROA Technologies, Gainesville, FL*

NANOMATERIALS
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TP 528 **Surface-assisted Laser Desorption/Ionization Time-of-Flight Mass Spectrometry of Small Biomolecules and Asphaltenes Using Transition Metal Oxide Nanoparticles**; Abayomi Olaitan[1]; Lauren F. Barnes[1]; Joseph R. Yount[1]; Savanna Ward[1]; Bryan Zanca[1]; Karen S. Molek[1]; *[1]University of West Florida, Pensacola, Florida*

TP 529 **Field-Flow Fractionation (FFF) Coupled with ICP-MS for Characterization of Metallic Nanoparticles in Tattoo Ink, and FFF-spICP-MS Analysis of Gold Nanoparticles**; Robert Reed[1]; Soheyl Tadjiki[1]; Florian Meier[2]; Tony Pfaffe[2]; Evelin Moldenhauer[2]; Thorsten Klein[2]; *[1]Postnova Analytics Inc., Salt Lake City, Utah; [2]Postnova Analytics GmbH, Landsberg am Lech, Germany*

TP 530 **Temperature and pH Alteration of Silver Nanoparticle Protein Corona Composition Studied by Quantitative Label-Free Proteomics**; Vladimir Gorshkov[1]; Julia A Bubis[2, 3]; Elizaveta M Solovyeva[2, 3]; Mikhail V Gorshkov[2, 3]; Frank Kjeldsen[1]; *[1]University of Southern Denmark, Odense, Denmark; [2]V. L. Talrose Institute for Energy Problems of Chemical Physics, Russian Academy of Sciences, Moscow, Russia; [3]Moscow Institute of Physics and Technology (State University), Dolgoprudnyj, Russia*

TP 531 **Development of Antibody Decorated Magnetic Nanoparticles for the Assay of Abused Drug in Urine**; Kun-Ru Wu[1]; He-Hsuan Hsiao[1]; *[1]NCHU, Department of Chemistry, Taichung, Taiwan*

TP 532 **Surface Chemistry Analysis of Bio-Conjugated Gold Nanoparticles by LDI/MALDI-(CID)-FTICR MS**; Fabrizio Chiodo[1, 2]; Yuri E.M. van der Burgt[1]; Jeroen D. Codée[2]; Manfred Wuhrer[1]; Cornelis H. Hokke[1]; Simone Nicolardi[1]; *[1]Leiden University Medical Center, Leiden, Netherlands; [2]Leiden University, Leiden, Netherlands*

TP 533 **Analysis of Fungal Epipolythiodioxopiperazine Alkaloids' Encapsulated within Expansile Nanoparticles *via* UPLC- MS-MS/MS**; Chiraz Soumia Amrine[1]; Aaron H Cobly[2]; Mark W Grinstaff[2]; Joanna E Burdette[3]; Daniel A Todd[1]; Cedric J Pearce[4]; Nicholas H Oberlies[1]; *[1]University of North Carolina at Greensboro, Greensboro, NC; [2]Boston University, Boston, Massachusetts; [3]University of Illinois, Chicago, Illinois; [4]Mycosynthetix, Inc, Hillsborough, NC*

TP 534 **Molecular Analysis of Neurons from Single Ganglia of *Lymnaea stagnalis* by MALDI and Nanophotonic Laser Desorption Ionization Mass Spectrometry**; Nikkita Khattar[1]; Linwen Zhang[1]; Zita Zrinyi[2]; Zsolt Pirger[2]; Akos Vertes[1]; *[1]The George Washington University, Washington, DC; [2]Balaton Limnological Institute, Tihany, Hungary*

TP 535 **Analysis of Microorganism Extracts by Laser Desorption Ionization Mass Spectrometry from Silicon Nanopost Arrays**; Jarod Fincher[1]; Akos Vertes[1]; *[1]The George Washington University, Washington, DC*

TP 536 **Surface Modified and Derivatized Silicon Nanopost Arrays for Increased Molecular Coverage and Sensitivity by Laser Desorption Ionization Mass Spectrometry**; Jacqueline E. Dyer[1]; Jarod A. Fincher[1]; Rachelle S. Jacobson[1]; Nicholas J. Morris[2]; Matthew J. Powell[2]; Akos Vertes[1]; *[1]The George Washington University, Washington, DC; [2]Protea Biosciences, Morgantown, WV*

NUCLEIC ACIDS AND OLIGONUCLEOTIDES I
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TP 537 **ESI and CAD MS Studies of Fe(II) Binding to RNA Mononucleotides**; Giovanni Calderisi[1]; Kathrin Breuker[1]; *[1]University of Innsbruck, Innsbruck, Tirol*

TP 538 **TiO2-Based Solid Phase Extraction and LC-Coupled Mass Spectrometry for the Detection of 2'-O-methylmodifications in tRNA**; Manasses Jora[1]; Robert Ross[1]; Patrick A. Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH*

TP 539 **LC-MS Based Detection of Radiation Induced Effects on RNA and Its Chemical Modifications**; Congliang Sun[1]; Patrick A Limbach[1]; Balasubrahmanyam Addepalli[1]; *[1]University of Cincinnati, Cincinnati, OH*

TP 540 **Quantitation of siRNA in Biological Matrices by Liquid Chromatography and High Resolution Accurate Mass Spectrometry (LC/MS-HRAM)**; Ju Liu[1]; Krishna Aluri[1]; Vikrant Gohil[1]; Chris Tran[1]; Jing Li[1]; Samuel Wainhaus[1]; Yuanxin xu[1]; *[1]Alnylam Pharmaceuticals, Cambridge, MA*

TP 541 **Identification of Post-Transcriptional Modifications of tRNAs in Archaeal Organisms Using Liquid Chromatography and Mass Spectrometry**; Ningxi Yu[1]; Patrick A. Limbach[2]; *[1]University of Cincinnati, Cincinnati, Ohio; [2]University of Cincinnati, Cincinnati , OH*

TP 542 **Improving MS Sensitivity through the Reduction of Metal Salt Adducts in IP-RPLC/MS Oligonucleotide Analyses**; Robert Birdsall[1]; Martin Gilar[2]; Joe Fredette[2]; Ying Qing Yu[2]; Weibin Chen[2]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Milford, MA*

TP 543 **Impurity Profiling Second Generation Therapeutic Oligonucleotides Using Liquid Chromatography Mass Spectrometry**; Noha Morsy ElZahar[1]; Nancy Magdy[2]; Amira M. El-Kosasy[2]; Michael G. Bartlett[1]; *[1]Department of Pharmaceutical and Biomedical Sciences, College of Pharmacy, The University of Georgia, Athens, GA; [2]Pharmaceutical Analytical Chemistry Department, Faculty of Pharmacy, Ain Shams University, Cairo, Egypt*

TP 544 **Characterization of Amino Acid-Linked Platinum Adducts to RNA *via* Tandem Mass Spectrometry**; Chenchen He[1]; Bett Kimutai[1]; Lucas A. Hamlow[1]; Yanlong Zhu[1]; Harrison A. Roy[1]; Jun Jiang[1]; Xun Bao[1]; C. S. Chow[1]; Jonathan Martens[2]; Juehan Gao[2]; Giel Berden[2]; Jos Oomens[2]; M. T. Rodgers[1]; *[1]Wayne State University, Detroit, MI; [2]FELIX Facility, Radboud University, Netherlands*

TP 545 **Characterization of Post-Transcriptional Modifications Using Low-Mass-Fragment Signatures Generated by Highly-Accurate Tandem Mass Spectrometry**; Hiroshi Nakayama[1]; Yuko Nobe[2]; Yoshio Yamauchi[2]; MASATO TAOKA[2]; Toshiaki Isobe[2]; *[1]RIKEN Center for Sustainable Resource Science, Wako, Japan; [2]Department of Chemistry, Tokyo Metropolitan Univ., Tokyo, Japan*

TP 546 **Characterization of Intramolecular Nucleobase-Phosphate Interactions by Site-Specific Nucleobase Methylation and Collisionally Activated Dissociation**; Heidelinde Glasner[1]; Christian Riml[1]; Christoph

Falschlunger[1]; Ronald Micura[1]; Kathrin Breuker[1]; *[1]University of Innsbruck, Innsbruck, Austria*

TP 547 **Identification of a Novel Deaminated Metabolite on a Single-Stranded Oligonucleotide, in Monkey Liver by HPLC and High-Resolution Mass Spectrometry**; Jing Li[1]; Ju Liu[1]; Samuel Wainhaus[1]; Yuanxin Xu[1]; *[1]Alnylam Pharmaceuticals, Cambridge, MA*

TP 548 **Two Quantitative Assays for the Phosphorodiamidate Morpholino Oligomer (PMO)SRP-4045 in MousePlasma using HPLC-MS/MS Coupled with Solid Phase Micro-Extraction**; AIHUA LIU[1]; Jiangbo Zhang[2]; Nan Zhao[1]; Shawn Burton[1]; Michael Carver[2]; Sherry Liu[1]; Joseph Rutkowoski[1]; Scott Reuschel[1]; Min Meng[1]; *[1]Covance, Salt Lake City, UT; [2]Sarepta Therapeutics, Inc., Cambridge, MA*

TP 549 **Metal Ion-, Base-, and Acid-Catalyzed Hydrolysis of Total Yeast RNA for Kendrick Mass Analysis of Posttranscriptionally Modified Nucleotides**; Matthias Halper[1]; Kathrin Breuker[1]; *[1]University of Innsbruck, Innsbruck, Austria*

TP 550 **Characterization of Metallocene-Oligonucleotide Adducts with Different Activation Techniques**; Rahel Eberle; *University of Bern, Bern, Switzerland*

TP 551 **Novel Cytidine Specific Ribonuclease for MS-Based RNA Modification Mapping**; Priti Thakur[1]; Patrick A. Limbach[1]; Balasubrahmanyam Addepalli[1]; *[1]University of Cincinnati, Cincinnati , OH*

TP 552 **Untargeted Metabolomic Profiling of the Epitranscriptome: Discovery of New Modified Nucleobases in RNA**; Megan R Showalter[1]; Tomas Cajka[1]; Nont Kosaisawe[1]; Kacey VanderVorst[2]; Kermit L Carraway III[2]; Oliver Fiehn[1]; *[1]NIH West Coast Metabolomics Center, University of California Davis, Davis, CA; [2]Department of Biochemistry and Molecular Medicine, UC Davis, Sacramento, CA*

TP 553 **Identification of YTHDF2 as a Reader for 5-Methylcytosine in RNA**; Xiaoxia Dai[1]; Lin Li[1]; Jie Li[2]; Gwendolyn Gonzalez[1]; Changjun You[1]; Weili Miao[1]; Junchi Hu[3]; Lijuan Fu[1]; Yanhui Xu[2]; Weifeng Gu[1]; Yinsheng Wang[1]; *[1]UC Riverside, Riverside, CA; [2]Fudan University, Shanghai, China; [3]Shanghai Institute of Materia Medica, Shanghai, Shanghai*

TP 554 **LC-MS/MS for the Investigation of the Altered Levels of 5-HmdC in Cancer Cells**; Yang Yu[1]; Yinsheng Wang[1]; *[1]UC Riverside, Riverside, CA*

TP 555 **Novel Fluorescently-Labeled Nucleotide Triphosphates - Incorporation with different DNA polymerases: MALDI MS Perspective**; Igor P. Smirnov[1]; Galina E Pozmogova[1]; Alexandr V Chudinov[2]; Edward N Timofeev[2]; *[1]Institute of Physico-Chemical Medicine, Moscow, Moscow; [2]Engelhardt Institute of Molecular Biology, Moscow, Russia*

TP 556 **Evaluation of RNase U2 Variants By Mass Spectrometry for the Improvement of RNA Modification Mapping**; Beulah Mae Ann Solivio[1]; Balasubrahmanyam Addepalli[1]; Patrick A. Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH*

PROTEINS: GENERAL AND MEMBRANE
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TP 557 **Investigating Protein Interactions of MALAT-1, a Long-Noncoding RNA, in Brain Tumors**; Maike Langini[1, 2, 3]; Nan Qin[2, 3, 4]; Daniel Picard[2, 3, 4]; Anja Stefanski[1, 5]; Kai Stühler[1, 5]; Marc Remke[2, 3, 4]; *[1]Institute of Molecular Medicine, University Hospital Duesseldorf, Duesseldorf, Germany; [2]Department of Pediatric Oncology, Hematology and Clinical Immunology, University Hospital Duesseldorf, Duesseldorf, Germany; [3]Division of Pediatric Neuro-Oncogenomics, German Cancer Consortium and German Cancer Research Center - partner site Essen/Duesseldorf, Duesseldorf, Germany; [4]Department of Neuropathology, Heinrich Heine University Duesseldorf, Duesseldorf, Germany; [5]Molecular Proteomics Laboratory, BMFZ, Heinrich Heine University, Duesseldorf, Germany*

TP 558 **Photoaffinity Probes and Quantitative Proteomics Enable Assessment of Target Engagement and Compound Potency in Live Cells**; Christian Eberl[1]; Johanna Vappiani[1]; Anne J. Wagner[1]; Stephanie Lehmann[1]; Marcel Muelbaier[1]; Marcus Banscheff[1]; *[1]Cellzome, Heidelberg, BW*

TP 559 **Revisiting Ethanol Precipitation of Plasma Proteins to Deplete Albumin and Increase Depth of Coverage**; Nicholas J. Carruthers[1]; Paul Stemmer[2]; Joseph A. Caruso[2]; *[1]Wayne State University, Detroit, MI; [2]Wayne State University, Detroit, MI*

TP 560 **Alpha-Lytic Protease Digestion of Proteins: Comparison with Trypsin and Subtilisin**; Colleen McClung[1]; Christopher J Noren[1]; Cristian I. Ruse[1]; *[1]New England BioLabs, Ipswich, MA*

TP 561 **Cell Surface Thermal Proteome Profiling Enables Monitoring the Interactions of Small Molecules and Endogenous Ligands with the Plasma Membrane Proteome**; Mathias Kalxdorf[1]; Ina Tögel[1]; Christian Eberl[1]; Marcus Bantscheff[1]; *[1]Cellzome, a GSK company, Heidelberg*

TP 562 **Characterization of Degradation Profile of Collagen in Archaeological Specimens by Mass Spectrometry**; Mao Karino[1]; Kazuki Kawahara[2]; Seiji Kadowaki[3]; Yoko Taniguchi[4]; Akira Tsuneki[4]; Mehdi Moini[5]; Takashi Nakazawa[1]; *[1]Nara Women's University, Nara, Japan; [2]Osaka University, Suita, Japan; [3]Nagoya University Museum, Nagoya, Japan; [4]University of Tsukuba, Tsukuba, Japan; [5]George Washington University, Washington, DC*

TP 563 **Comparative Microsomal Proteomics of the NCI-H23 Lung Cancer Cell Line Grown in 2D and 3D Culture**; Jan A. Kaczmarczyk[1]; Rhonda R. Roberts[1]; Richard G. Saul[1]; John J. Gildea[2]; Robin A. Felder[3]; Gordon R. Whiteley[1]; Josip Blonder[1]; *[1]Frederick National Laboratory for Cancer Research (FNLCR), Leidos Biomedical Research Inc., Frederick , MD; [2]Omic Labs, Scottsville, VA; [3]Department of Pathology, University of Virginia School of Medicine, Charlottesville, VA*

TP 564 **Mass Spectrometry Based Identification, Quantitation, and Characterization of Novel Cell Surface Markers of Human Cardiomyocytes**; Matthew Waas[1]; Ted Keppel[1]; Chelsea Fujinaka[1]; Ranjuna Weerasekera[1]; Rebekah Gundry[1]; *[1]Medical College of Wisconsin, Milwaukee, WI*

TP 565 **Discovery and Quantitation of Cell Surface Proteins during Pluripotent Stem Cell-Derived Cardiomyocyte Differentiation and Maturation**; Chelsea Fujinaka[1]; Ted Keppel[1]; Matthew Waas[1]; Rebekah Gundry[1]; *[1]Medical College of Wisconsin, Milwaukee, WI*

TP 566 **The Quantification of Low Abundance Host Cell Protein Impurities by Standard Addition Mass Spectrometry Method**; Feng Yan[1]; Zihao Wang[1]; *[1]GSK Vaccines, Rockville, MD*

TP 567 **Protease Networks and Proteostasis in Plant Chloroplasts and Mitochondria; an Omics Approach to Organellar Protein Maturation, Stability and Turnover**; Klaas J. Van Wijk[1]; Elden Rowland[2]; Kristina Majsec[2]; Giulia Friso[1]; Nazmul H. Bhuiyan[2]; Jitae Kim[2]; Vivek Kumar[3]; Sunita Kumari[3]; Doreen Ware[3]; Qi Sun[2]; *[1]Cornell University, Ithaca, New York; [2]Cornell University, Ithaca, New York; [3]Cold Spring Harbor laboratory, Cold Spring Harbor, NY*

TP 568 **Multiplexed Mass Spectrometric Screening of EGFR Mutations in Non-small-cell Lung Cancer**; Chi-Ting Lai[1]; Wai-Kok Choong[2]; T. Mamie Lih[2]; Hui-Yin Chang[2]; Ting-Yi Sung[2]; Hsuan-Yu Chen[3]; Yu-Ju Chen[4]; Chia-Li Han[5]; *[1]Genome and Systems Biology Degree Program,*

National Taiwan University, Taipei, Taiwan; [2]Institute of Information Science, Academia Sinica, Taipei, Taiwan; [3]Institute of Statistical Science, Academia Sinica, Taipei, Taiwan; [4]Institute of Chemistry, Academia Sinica, Taipei, Taiwan; [5]Master Program for Clinical Pharmacogenomics and Pharmacoproteomics, Taipei Medical University, Taipei, Taiwan

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TP 569 **Development of a Method for the Determination of α-Tubulin Acetylation by Immunopurification–Multiple Reaction Monitoring Mass Spectrometry (IP-MRM-MS)**; Xiangkun Yang[1]; Michael Bartlett[1]; *[1]University of Georgia, Athens, Georgia*

TP 570 **2D-Immunoblotting Combined with High-Resolution Mass Spectrometry Reveals a Novel Phosphorylation Site in Cofilin-1 Involved in Cardiomyopathy**; Solenne Chardonnet[1]; Maria Chatzifrangkeskou[2]; Yannick Tanguy[2]; Thibault Marais[2]; Howard J. Worman[3, 4]; Gisèle Bonne[2]; Antoine Muchir[2]; *[1]Sorbonne Universités, UPMC Univ Paris 06, Inserm, UMS Omique, Plateforme P3S, Paris, France; [2]Center of Research in Myology, UPMC-INSERM UMR974, CNRS FRE3617, Paris, France; [3]Department of Medicine, College of Physicians and Surgeons, Columbia University, New York, NY; [4]Department of Pathology and Cell Biology, College of Physicians and Surgeons, Columbia University,, New York, NY*

TP 571 **Development of a High-throughput Method to Identify Disulfidesin Human Recombinant Soluble Guanylyl Cyclase**; Chuanlong Cui[1]; Lin Yan[1]; Annie Beuve[2]; Hong Li[1]; *[1]Center for Advanced Proteomics Research, Rutgers New Jersey Medical School, Newark, NJ; [2]Department of Pharmacology, Physiology and Neuroscience, Rutgers New Jersey Medical Shool, Newark, NJ*

TP 572 **Highly Efficient and Reproducible Online 2D-LC Method for Determination of Glycated Peptides**; Lina Zhang[1]; Chih-Wei Liu[1]; Qibin Zhang[1, 2]; *[1]Center for Translational Biomedical Research, Kannapolis, NC; [2]University of North Carolina at Greensboro, Greensboro, NC*

TP 573 **Characterization of Disulfide Linkages in Proteins by Ultraviolet Photodissociation (UVPD)**; Montana Quick[1]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

TP 574 **Reprogramming the SNO-Proteome in the brain of the Shank3-KO Model of Autism Spectrum Disorder**; Haitham Amal[1]; Vadiraja Bhat [2]; John S. Wishnok[1]; Guoping Feng[3]; Steven R. Tannenbaum[1, 3]; *[1]Massachusetts Institute of Technology, Cambridge, MA; [2]Agilent Technologies, Wilmington , DE; [3]McGovern Institute for Brain Research, Cambridge, MA*

TP 575 **Succinyl-CoA Potentially Regulates the Oligomeric Forms of Cyanobacterial Citrate Synthase through Succinylation**; John Muroski[1]; Hong Nguyen[1]; Joseph A. Loo[1]; Rachel R. Ogorzalek Loo[1]; *[1]UCLA, Los Angeles, CA*

TP 576 **Comprehensive Profiling of Lysine Modifications in Biosilica-Associated Proteome**; Alexander Milentyev[1]; Christoph Heintze[2]; Nicole Poulsen[2]; Nils Kröger[2, 3]; Andrej Shevchenko[1]; *[1]MPI-CBG, Dresden, Germany; [2]B-CUBE Center for Molecular Bioengineering, Dresden, Germany; [3]Department of Chemistry and Food Chemistry, Technische Universität Dresden, Dresden, Germany*

TP 577 **Automated Proteome-Wide Data Analysis Strategies for the "Unbiased" Detection of Dityrosine Cross-Linked Proteins Indicative of Oxidative Stress in Neurodegenerative Diseases**; Eugene A Kapp[1]; Soumya Mukherjee[2]; Blaine R Roberts[1]; *[1]The Florey, Melbourne, Australia; [2]Indian Association for the Cultivation of Science, Jadavpur, India*

TP 578 **Symmetric Dimethylated Arginines Residues in Proteins from Human Lung Cancer Cells**; Stephanie Lehman[1]; Hongshan Chan[2]; Dina L Bai[3]; Jeffrey Shabanowitz[3]; Donald F Hunt[3]; David Shechter[4]; *[1]University of Virginia, Charlottesville, VA; [2]Nanjing Medical University, Nanjing, China; [3]University of Virginia, Charlottesville, VA; [4]Albert Einstein College of Medicine, New York, NY*

TP 579 **Identification and Selective Enrichment of Functional Arginine Residues Using Bio-Orthogonal Click Chemistry and Mass Spectrometry**; Maheshika S.K. Wanigasekara[1]; Abu Hena M Kamal[1]; Saiful M. Chowdhury[1]; *[1]University of Texas at Arlington, Arlington, TX*

TP 580 **Proteome-Wide Acetylation Dynamics Revealed by Metabolic Labeling and Quantitative Proteomics**; Yekaterina Kori[1]; Simone Sidoli[1]; Zuo-Fei Yuan[1]; Peder J. Lund[1]; Xiaolu Zhao[2]; Benjamin A. Garcia[1]; *[1]Epigenetics Program, Department of Biochemistry and Molecular Biophysics, University of Pennsylvania School of Medicine, Philadelphia, PA; [2]Wuhan University, Wuhan, China*

TP 581 **Site-specific N-Glycosylation Mapping for Glycopeptides in the Presence of Additional Unknown Post-Translational Modifications (II) by Y1 (Peptide + HexNAc) Ion**; Benlian Wang[1, 2]; David Salom[3, 4]; Krzysztof Palczewski[3]; Mark R. Chance[1, 2]; *[1]Center for Proteomics and Bioinformatics, Case Western Reserve University, Cleveland, OH; [2]Department of Nutrition, Case Western Reserve University, Cleveland, OH; [3]Department of Pharmacology, Case Western Reserve University, Cleveland, OH; [4]Polgenix, Inc., Cleveland, OH*

TP 582 **Reversible Phosphorylation of the RVSF Motif in PP1 Regulatory Proteins by Aurora B Controls PP1 Docking During the Cell Cycle**; Isha Nasa[1, 2]; Scott Rusin[1]; Arminja Kettenbach[1]; Greg Moorhead[2]; *[1]Department of Biochemistry, Dartmouth College, Lebanon, NH; [2]University of Calgary, Calgary, AB*

TP 583 **Strategies for Enriching and Identifying the Farnesyl Peptide from Complex Sample Using Mass Spectrometry**; Zixiang Fang[1]; Saiful M. Chowdhury[1]; *[1]University of Texas at Arlington, Arlington, TX*

TP 584 **Identification of Novel E3 SUMO Ligase PIAS1 Substrates by Quantitative Proteomics**; Chongyang Li[1]; Francis McManus[1]; Pierre Thibault[1]; *[1]IRIC-Université de Montréal, Montréal, QC*

TP 585 **Dynamic Mapping of Glyco-Conjugates in Human Prefrontal Cortex *via* Neuroglycomic Approach Reveals Age- and Region-Specific Biosynthetic Pathway**; Jua Lee[1, 2]; Sumin Kim[1, 2]; Sureyya Ozcan[3]; Sabine Bahn[3]; Hee-Sup Shin[4]; Hyun Joo An[1, 2]; *[1]Asia Glycomics Reference Site, Chungnam National University, South Korea; [2]Graduate School of Analytical Science and Technology, Chungnam National University, South Korea; [3]Institute of Biotechnology, University of Cambridge, UK; [4]Center for Cognition and Sociality, Institute for Basic Science, South Korea*

TP 586 **Top-Down Mass Spectrometry Reveals the Impact of Cardiac Tissue Handling on Myofilament Protein PTMs**; Wenxuan Cai[1]; Beini Lyu[2]; Zachary L Hite[3]; Zhijie Wu[3]; Ziqing Lin[2]; Zachery R Gregorich[2]; Takushi Khomoto[2]; Ying Ge[2, 3]; *[1]University of Wisconsin-Madison, Madison, WI; [2]University of Wisconsin Madison, Madison, WI; [3]University of Wisconsin - Madison Department of Chemistry, Madison, WI*

TP 587 **Direct and Indirect Analysis of S-Palmitoylated Proteins in Ocular Lens by Mass Spectrometry** ; Zhen Wang[1]; Kevin L. Schey[2]; *[1]Vanderbilt University, Nashville, TN; [2]Vanderbilt University, Nashville, TN*

TP 588 **Probing the Deleterious Effects of Protein Aging by Tracking Isomerization in the Human Eye Lens**; Yana Lyon[1]; Ryan R Julian[2]; *[1]University of California, Riverside, Riverside, CA; [2]UC Riverside, Riverside, CA*

TP 589 **Regulation of RNA Polymerase II Transcription Elongation by Ubiquitylation**; Sarah Peck[1]; Melanie J. Fox[1]; Whitney R. Smith-Kinnaman[1]; Lea Morical[1]; Hongyu Gao[1]; Yunlong Liu[1]; Amber L Mosley[1]; *[1]Indiana University School of Medicine, Indianapolis, IN*

TP 590 **Expanding OxcyscPILOT to Study SNO and S-acyl in Aging Brain**; Ryan R Dyer[1]; Renã A.S. Robinson[1]; *[1]University of Pittsburgh, Pittsburgh, PA*

TP 591 **Moneyball for PTMs: The Science of Winning the Unfair Game of Functional PTM Prognostication**; Matthew P Torres[1]; Henry M Dewhurst[1]; *[1]School of Biological Sciences, Georgia Institute of Technology, Atlanta, GA*

TP 592 **Serotransferrin Glycation and Ceruloplasmin Deamidation Result in their Increased Degradation in Type 2 Diabetes**; Makan Golizeh[1]; Kwangwon Lee[2]; Serguei Ilchenko[2]; Abdullah Osme[2]; James Bena[3]; Rovshan Sadygov[4]; Takhar Kasumov[2]; *[1]Northeast Ohio Medical University, Rootstown, Ohio; [2]Northeast Ohio Medical Univeristy, Rootstown, Ohio; [3]Cleveland Clinic Foundation, Cleveland, Ohio; [4]University of Texas Medical Branch, Galveston, TX*

TP 593 **Convenient Strategy for Mapping N-Glycosylation Sites Using Microwave-Assisted Acid Hydrolysis**; Cheng Ma[1]; Peng George Wang[2]; *[1]Georgia state university, Atlanta, GA; [2]GSU, Atlanta, GA*

TP 594 **Elucidating the Role of Histone H4 Lysine 79 Monomethylation in Chlamydomonas reinhardtiiusing Top Down Mass Spectrometry and RNA interference**; Jack W Clemmensen[1]; Aliyya Khan[1]; Anthony T. Iavarone[2]; Gary H. Karpen[3]; James Pesavento[1]; *[1]Saint Mary's College of California, Moraga, CA; [2]QB3/Chemistry Mass Spectrometry Facility, University of California, Berkeley, CA; [3]Lawrence Berkeley National Laboratory, Berkeley, CA*

TP 595 **Construct N-Glycan Databases for Glycoproteomics by Using a Canonical String Representation**; Xiao-Jin Zhang[1]; Wen-Feng Zeng[1]; Jian-Qiang Wu[1]; Yang Zhang[2]; Ming-Qi Liu[2]; Pan Fang[2]; Peng-Yuan Yang[2]; Si-Min He[1]; *[1]Institute of Computing Technology, Beijing, Beijing; [2]Fudan University, Shanghai, Shanghai*

TP 596 **Quantitative Analysis of Phosphotyrosine Signaling Reveals the Differential Mechanism of Mutated Granulocyte-Colony Stimulating Factor Receptors (G-CSFRs) Leading to Leukemia**; Pankaj Dwivedi[1]; David E Muench[2]; Mohammad Azam[2]; H. Leighton Grimes[2]; Kenneth D Greis[1]; *[1]University of Cincinnati, Cincinnati, OH; [2]Cincinnati Children's Hospital Medical Center, Cincinnati, OH*

TP 597 **Mass Spectrometry-Based Analysis of an Emerging Post-Translational Modification, AMPylation, and its Role in Molecular Signaling**; Kelly Servage[1]; Amanda Casey[1]; Junmei Zhang[1]; Kim Orth[1]; *[1]UT Southwestern, Dallas, TX*

TP 598 **Histone Epigenetic Changes in Response to Chronic Methamphetamine Abuse**; Lisa M Orr[1]; Molly H Tibbs[1]; Chris Bolden[1]; Eric C Peterson[1]; Alan J Tackett[1]; *[1]University of Arkansas for Medical Sciences, Little Rock, AR*

TP 599 **Detection of a Phosphorylated Glycine-Serine Linker in an IgG-Based Fusion Protein Using CID, EThcD, HCD, Peptide Spiking and Alkaline Phosphatase**; Bjoern Mautz[1]; Oksana Tyshchuk[1]; Hans Rainer Voelger[1]; Claudia Ferrara Koller[2]; Patrick Bulau[3]; Hans Koll[1]; Michael Molhoj[1]; *[1]Roche Pharma Research and Early Development (pRED), Large Molecule Research, Roche Innovation Center Munich, Penzberg, Germany; [2]Roche Pharma Research and Early Development (pRED), Discovery Oncology, Roche Innovation Center Zurich, Schlieren, Switzerland; [3]Roche Pharma Technical Development Penzberg, Penzberg, Germany*

TP 600 **Characterization of Post Translational Modifications of Light Exposed IgG1—Assay Optimization and Cross-Validation with Four Serine-Proteinases Digestions**; Yao Chen[1]; Anuja Ganesan[1]; Victor Vinci[1]; Yunsong Li[1]; *[1]COOK PHARMICA, Bloomington, IN*

TP 601 **Charge State Distribution Modification as a Mechanism to Reduce Apparent Complexity of an Intact Fusion Protein Therapeutic**; Matthew D Maust[1]; Katy Ryan[1]; Heather Anderson[1]; Harsha Gunawardena[2]; Andrew Mahan[2]; Eric Beil[2]; Hirsh Nanda[2]; *[1]Protea Biosciences, Morgantown, West Virginia; [2]Janssen Pharmaceuticals R&D, Spring House, PA*

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TP 602 **Discovery-Based Proteomics Identifies Molecular Signatures Associated with Hydrosalpinx** ; Elizabeth Yohannes[1]; Avedis Kazanjian[2]; Gregory Chow[3]; Ronald Beesley[4]; Ryan Heitmann[3]; Richard Burney[3, 5]; *[1]Department of Clinical Investigation, MADIGA Army Medical Center, 9040 Jackson Ave., Tacoma, WA; [2]Department of Clinical Investigation, MADIGAN Army Medical Center, 9040 Jackson Ave., Tacoma, WA; [3]Department of Obstetrics and Gynecology, Division of Reproductive Endocrinology and Infertility, MADIGAN Army Medical Center, 9040 Jackson Ave, Tacoma, WA; [4]Department of Obstetrics and Gynecology, Division of Reproductive Endocrinology and Infertility, MADIGAN Army Medical Center, 9040 Jackson Ave, Tacoma, US; [5]Department of Clinical Investigation, MADIGAN Army Medical Center, 9040 Jackson Ave, Tacoma, WA*

TP 603 **Exploring Proteins Expressed Exclusively within the Inner Ear Hair Cells as Potential Drivers of Deafness**; Miguel Ramirez[1]; Ann E. Hickox[1]; Ann C.Y. Wong[2, 3]; Kwang Pak[2]; Chelsee Strojny[1]; Allen F Ryan[2]; Jeffrey N Savas[1]; *[1]Northwestern University Feinberg School of Medicine, Chicago, Illinois; [2]University of California, San Diego, La Jolla, CA; [3]University of New South Wales, Sydney, Australia*

TP 604 **10-plex TMT Label-based Quantitative MS2 and MS3 Proteomic Analysis of Hypertriglyceridemia-induced Brain Microvascular Lipotoxic Injury**; Anthony W Herren[1]; Tun Nyunt[2]; Brett S Phinney[1]; John C Rutledge[2]; Hnin H Aung[2]; *[1]University of California, Davis, Genome Center, Davis, CA; [2]University of California, Davis, School of Medicine, Internal and Cardiovascular Medicine, Davis, CA*

TP 605 **Application of Scheduled GeLC-MRM Method for High-throughput Screening of Small GTPases Involved in Colon Cancer Metastasis**; Ming Huang[1]; Yinsheng Wang[1]; *[1]University of California, Riverside, CA*

TP 606 **Hepatic Mitochondrial Dysfunction in a Mouse Model of NASH is Associated with Increased Degradation of Mitochondrial Proteins**; Kwangwon Lee[1]; Abdullah Osme[1]; Makan Golizeh[1]; Serguei Ilchenko[2]; Mahbubur Rahman[3]; Rovshan Sadygov[3]; Takhar Kasumov[1]; *[1]Northeast Ohio Medical Univeristy, Rootstown, Ohio; [2]Northeast Ohio Medical Univeristy, Rootstown, OH; [3]University of Texas Medical Branch, Galveston, TX*

TP 607 **Dynamic Changes of Ca2+-Mediated Signalosome by Exposure to High-Glucose Dependent Short-Term Time-Course in the Nuclear Proteome of Pancreatic B-Cells**; Taewook Kang[1]; Pia Jensen[1]; Martin Røssel Larsen[1]; *[1]Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense, Denmark*

TP 608 **Changes in Mitochondrial Proteins, Metabolites, and Protein Acylation in Response to Macronutrient Stresses in the Mouse Liver** ; Jesse G. Meyer[1]; Natan Basisty[1]; Samir Softic[2]; Guoxiao Wang[2]; BIRGIT SCHILLING[1]; Christopher Newgard[3]; C. Ronald Kahn[2];

Bradford W Gibson[1, 4]; [1]*Buck Institute for Research on Aging, Novato, CA;* [2]*Joslin Diabetes Center, Harvard Medical School, Boston, MA;* [3]*Sarah W. Stedman Nutrition and Metabolism Center, Duke University School of Medicine, Durham, NC;* [4]*Amgen, Thousand Oaks, CA*

TP 609 **Label Free Quantitative Proteomics Analysis Reveals the Pathways Involved in Factor VIII Secretion by the Bradykinin Activated Mouse Dendritic Cells**; Cristina Clement[1]; Monika Dzieciatkowska[2]; Antonia Follenzi[3]; [1]*Albert Einstein College of Medicine, Bronx, NY;* [2]*University of Colorado Denver, Denver, Colorado;* [3]*School of Medicine, University of Piemonte Orientale, Novara, Italy*

TP 610 ***Methanosarcina mazei, acetivorans*, and *barkeri* Proteomic Responses to Different Methylotrophic Substrates**; Deborah A. Jarrett[1]; Farzaneh Sedighian[1]; Hong Hanh Nguyen[1]; Robert P. Gunsalus[1]; Joseph A. Loo[1]; Rachel O. Loo[1]; [1]*University of California, Los Angeles, Los Angeles, CA*

TP 611 **Comparative Proteomic Analysis of Charcoal-Stripped Fetal Bovine Serum Revealed Modified Insulin-Like Growth Factor Signaling Responsiveness**; CHENGJIAN TU [1]; Michael Fiandalo[2]; Jun Li[1]; Jun Qu[1]; Li Tang[2]; James L. Mohler[2]; Yue Wu[2]; [1]*University at Buffalo, Buffalo, NY;* [2]*Roswell Park Cancer Institute, Buffalo, NY*

TP 612 **Pulse Isotopic Labeling Analysis Revealed Temporal Dynamics of Lysine Acetylation Proteome**; Tong Zhou[1]; Luke Erber[1]; Yue Chen[1]; [1]*University of Minnesota at Twin Cities, Minneapolis, MN*

TP 613 **Isobaric TMT 10-plex Labeled MultiNotch MS3 Analysis of Biological and Technical Variance in Human Uterine Smooth Muscle Tissue**; Craig Ulrich[1]; Christian Copley-Salem[1]; David Quilici[1]; Heather Burkin[1]; Iain Buxton[1]; Karen Schlauch[1]; [1]*University of Nevada, Reno, Reno, NV*

TP 614 **Quantitative Proteomic Analysis Applied to Differentiation of SH-SY5Y Human Neuroblastoma Cells as an *in vitro* Neuron-Like Model**; Jimmy Rodriguez[1]; Aniel Sanchez[2]; Livia Goto-Silva[3]; Fábio CS Nogueira[1]; Gilberto B Domont[1]; Magno Junqueira[1]; [1]*Federal University of Rio de Janeiro, Rio de Janeiro, Brazil;* [2]*Lund University, Lund, Sweden;* [3]*Instituto D'Or de Pesquisa e Ensino, Rio de Janeiro, Brazil*

TP 615 **Proteomic Profiles of H2S-regulated PTMs in Endothelial Cell under Hypoxia**; Xinggui Shen; *LSU Health-Shreveport, Shreveport, LA*

TP 616 **Identifying the Roles of ARMS2 and HTRA1 in the Pathogenesis of AMD Using Quantitative Functional Proteomics**; Joel D Federspiel[1]; Todd M Greco[2]; Pierre Jean Beltran[1]; Jim Handa[3]; Richard Semba[3]; Ileana M Cristea[1]; [1]*Princeton Universitry, Princeton, NJ;* [2]*Princeton University, Princeton, NJ;* [3]*Johns Hopkins University School of Medicine, Baltimore, MD*

TP 617 **Quantitative Discovery of the Alterations of the Human Kinome in Primary and Metastatic Melanoma Cells**; Weili Miao[1]; Lei Guo[1]; Yinsheng Wang[1]; [1]*University of California, Riverside, Riverside, CA*

TP 618 **Analysis of Proteome Degradation Kinetics with in vitro and *in vivo* Models of Alzheimer's Disease**; Timothy Hark[1]; Yi-Zhi Wang[1]; Samuel Smukowski[1]; Jeffrey N Savas[1]; [1]*Northwestern University, Chicago, IL*

TP 619 **Quantitative Proteomic Analysis of Cancer Cell Lines with Homozygous and Heterozygous Mutant KRAS Genotypes**; Josip Blonder[1]; Benjamin Orsburn[2]; Gordon R. Whiteley[1]; [1]*Frederick National Laboratory for Cancer Research (FNLCR), Leidos Biomedical Research Inc., Frederick , MD;* [2]*Thermo Fisher Scientific, West Palm Beach, Florida*

TP 620 **Comprehensive Analysis of Newly-Synthesized Protein Abundance Changes in Human Cells Stimulated with IGF1**; Ming Tong[1]; Haopeng Xiao[1]; Johanna Smeekens[1]; Ronghu Wu[1]; [1]*Georgia Tech , Atlanta, GA*

TP 621 **Dynamics of Zebrafish Heart Regeneration Using an HPLC-ESI-MS/MS Approach**; Danjun Ma[1]; Yuxi Yang[2]; Chengjian Tu[3]; Quanhu Sheng[4]; Xin Lou[2]; [1]*dongguan University of Technology, Dongguan, China;* [2]*Nanjing Medical University, Nanjing, China;* [3]*Department of Pharmaceutical Sciences, University at Buffalo, State University of New York, Buffalo, NY;* [4]*Department of Cancer Biology,vanderbilt university, Nashville, TN*

TP 622 **Quantitative Analysis of Two Cancer Signaling Pathways Using Multiplex-Immunoprecipitation and Targeted Mass Spectrometry**; Bhavin Patel[1]; Leigh Foster[1]; Penny Jensen[1]; Gregory Potts[1]; Abid Haseeb[1]; Kay Opperman[1]; Rosa Viner[2]; Andreas Huhmer[2]; John Rogers[1]; [1]*Thermo Fisher Scientific, Rockford, IL;* [2]*Thermo Fisher Scientific, San Jose, CA*

TP 623 **A Targeted Quantitative Proteomic Approach for Profiling Guanine Nucleotide-Exchange Factors during Cancer Metastasis**; Tianyu Qi[1]; Weili Miao[1]; Ming Huang[1]; Yinsheng Wang[1]; [1]*UC Riverside, Riverside, CA*

TP 624 **Analysis of Age-dependent Changes in the Proteome from *Drosophila melanogaster* Alzheimer's Disease Lines.**; Chris Brown[1]; Melissa A. Phelps[2]; Robert C. Eisman[2]; Jonathan Trinidad[2]; Thomas C. Kaufman[2]; David E Clemmer[2]; [1]*Indiana University, Bloomington , IN;* [2]*Indiana University Bloomington, Bloomington, IN*

TP 625 **Relative Quantification Using TMT11plex on a Modified Q Exactive HF Mass Spectrometer**; Tabiwang N. Arrey[1]; Rosa Viner[2]; Ryan D Bomgarden[3]; Eugen Damoc[4]; Markus Kellmann[4]; Thomas Moehring[4]; Alexander Harder[4]; [1]*Thermo Fisher Scientific, Bremen, Bremen;* [2]*ThermoFisher, San Jose, CA;* [3]*ThermoFisher Scientific, Rockford, Illinois;* [4]*Thermo Fisher Scientific, Bremen, Germany*

TP 626 **Development of a Novel Proteomics Approach to Investigate Cell Type-Specific Responses to Ethanol in Primary Glia and Neurons**; Jennifer Guergues[1]; Ashley E. Culver-Cochran[1]; Ping Zhang[2]; Bin Liu[2]; Stanley M Stevens[1]; [1]*University of South Florida, Tampa, FL;* [2]*University of Florida, Gainesville, FL*

TP 627 **Global Proteome Characterization of *Caenorhabditis elegans* Duaer Larvae**; Asifa K Zaidi[1]; Krishna Vukoti[1]; Masaru Miyagi [1]; [1]*Case Western Reserve Univers, Cleveland , OH*

TP 628 **Global Analysis of Secreted Proteins and Glycoproteins in *Saccharomyces cerevisiae***; Johanna Smeekens[1]; Haopeng Xiao[1]; Ronghu Wu[1]; [1]*Georgia Institute of Technology, Atlanta, GA*

TP 629 **Unbiased Discovery and Functional Confirmation of a Novel Target (DPP3) by Thermal Stability Label-Free Differential Mass Spectrometry (dMS)**; Steven Mullett[1]; Harris Bell-Temin[2]; Bennett Van Houten[2]; Wei Qian[2]; Andrey Bondarenko[3]; Mark Schurdak[4]; D. Lansing Taylor[4]; Andrew Stern[4]; Nathan A Yates[2]; [1]*University Of Pittsburgh, Pittsburgh, Pennsylvania;* [2]*University of Pittsburgh School of Medicine, Pittsburgh, PA;* [3]*Infoclinika, Seattle, WA;* [4]*Drug Discovery Institute, PIttsburgh, PA*

TP 630 **To TMT or LFQ, that is here the Question**; Jane M Liu[1]; Michael J Sweredoski[2]; Annie Moradian[2]; Sonja Hess[2]; [1]*Pomona College, Pomona, CA;* [2]*California Institute of Technology, Pasadena, CA*

TP 631 **Targeted Proteomics of Key Regulators of All-Trans Retinoic Acid During SIV Infection**; Wenjing Li[1]; Jianshi Yu[1]; Neil Sidell[2]; Maureen A Kane[1]; [1]*University of Maryland, Baltimore, Maryland;* [2]*Emory University, Atlanta, Georgia*

TP 632 **Strategies in Proteomic Quantification Using Isobaric Labeling: Insights from the Partiality of MS2 Reporter-ion Ratios**; Qiang Zhang[1]; Petra Erdmann-Gilmore[1]; Yiling Mi[2]; Rose Connors[2]; Sherri R. Davies[2]; Shunqiang Li[2]; Reid Townsend[2]; [1]*Washington University School of Medicine, St. Louis, MO;* [2]*Washington University School of Medicine, St. Louis, MO*

TP 633 **A Novel Cholesterol Mimetic Activity Based Proteomic Profiling (ABPP) Probe to Validate RORγt-LBD Target Engagement**; Aruna B. Wijeratne[1]; Jose M. Minguez[1]; Christian A. Clarke[1]; Timothy I. Richardson[1]; Thomas A. Engler[1]; Chalmers J. Michael[1]; *[1]Eli Lilly and Company, Indianapolis, IN*

TP 634 **Pushing the Limits: Boosting Sensitivity of PRM Assays for the Detection of Very Low Abundant Proteins in Complex Samples**; Emmanuelle Lezan[1]; Erik Ahrné[1]; Thomas Bock[1]; Alexander Schmidt[1]; *[1]PCF-Biozentrum-University of Basel, Basel, Switzerland*

TP 635 **MRM and PRM Assay Development for a Panel of >3,000 Proteins from 20 Mouse Tissues**; Sarah A. Michaud[1]; Nicholas J.T. Sinclair[1]; Ingo Feldmann[2]; Yassene Mohammed[1, 3]; Derek S. Smith[1]; Albert Sickmann[2]; Christoph H. Borchers[1, 4]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC; [2]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund, Germany; [3]Center for Proteomics and Metabolomics, Leiden University, Netherlands; [4]Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC*

TP 636 **Sequential Enrichment and Quantification of Phosphorylation on Reversibly Oxidized Proteoforms in *Chlamydomonas reinhardtii*.**; Leslie M. Hicks[1]; Evan W. McConnell[1]; Emily G. Werth[1]; *[1]UNC - Chapel Hill, Chapel Hill, NC*

TP 637 **Rapid and Accurate Instrumental Performance Gauge: Isotopologue Standards for Quality Control of LC-MS Platforms**; Alvaro Sebastian Vaca Jacome[1]; Gauthier Husson[1]; Alain Van Dorsselaer[1]; Christine Carapito[1]; *[1]IPHC, UdS, CNRS, UMR7178, Strasbourg, France*

TP 638 **Label Free Quantitative Proteomics Using Peptide Isotope Peak Intensities in Mass Spectrometry and Comparison of Label Free Methods**; Ki Na Yun[1, 2]; Gun Wook Park[1]; Ju Yeon Lee[1]; Eun Sun Ji[1]; Mee Jung Han[3]; Han Bin Oh[2]; Jong Shin Yoo[1]; Jin Young Kim[1]; *[1]Biomedical Omics Group, Korea Basic Science Institute, Ochang-eup, Cheongwon-gu, South Korea; [2]Department of Chemistry, Sogang University, 35 Baekbeom-ro, Mapo-gu, South Korea; [3]Department of Biomolecular and Chemical Engineering, Dongyang University, Yeongju, South Korea*

TP 639 **Quantitative Proteomics Comparison of Individual vs Pooled Biological Replicates**; Deanna Plubell[1]; Phillip A. Wilmarth[1]; Ashok P. Reddy[1]; Alexandra M. Fenton[1]; Jessica Minnier[1]; Larry L. David[1]; Nathalie Pamir[1]; *[1]Oregon Health & Science University, Portland, OR*

TP 640 **Activity-Based Profiling of Phosphoprotein Phosphatases by Mass Spectrometry-Based Proteomics**; Scott P. Lyons[1]; Isha Nasa[1]; Greg Moorhead[2]; Arminja Kettenbach[1, 3]; *[1]Department of Biochemistry and Cell Biology, Dartmouth College, Lebanon, NH; [2]University of Calgary, Calgary, AB; [3]Norris Cotton Cancer Center, Lebanon, NH*

TP 641 **Overclocking Multiplexed Proteomics: Millisecond Real-Time Searching Enables Data-Directed Quantitation**; Brian K Erickson[1]; Christopher Rose[1]; Julian Mintseris[1]; Derek Bailey[2]; Joao A Paulo[1]; Graeme McAlister[2]; Aleksandr Gaun[1]; Vlad Zabrouskov[2]; Steven P Gygi[1]; *[1]Harvard Medical School, Boston, MA; [2]Thermo Fisher Scientific, San Jose, CA*

TP 642 **Benchmarking Proteome Quantitation: Measuring the Small Writ Large**; Jeremy O'Connell[1]; Joao Paulo[1]; Jonathon O'Brien[1]; Steven Gygi[1]; *[1]Harvard Medical School, Boston, MA*

TP 643 **Multidimensional Tracking of GPCR Signaling *via* Peroxidase-Catalyzed (APEX) Proximity Labeling**; Marian Kalocsay[1]; Jaeho Paek[1]; Joao A Paulo[2]; Andrew Kruse[1]; Steven Gygi[1]; *[1]Harvard Medical School, Boston, MA; [2]Havard Medical School, Boston, MA*

TP 644 **A Quantitative Method for the Comparison of Mass Spectrometer Performance**; Sandra Spencer[1]; Eric Huang[2]; Neloni Wijeratne[2]; Oleg Silivra[2]; Claudia Martins[2]; Mary Blackburn[2]; Michael J MacCoss[1]; *[1]University of Washington Genome Sciences, Seattle, WA; [2]ThermoFisher, San Jose, CA*

TP 645 **There Are No Absolutes, Particularly in Protein Quantification**; Patricia L. Holland[1]; James J. Walters[2]; Kevin Ray[2]; Uma Sreenivasan[3]; Sarah Aijaz[3]; Russell P. Grant[1]; Christopher M. Shuford[1]; *[1]Laboratory Corporation of America, Burlington, NC; [2]MilliporeSigma, St. Louis, MO; [3]MilliporeSigma, Round Rock, TX*

TP 646 **Implementation of a Surrogate Cerebrospinal Fluid for use in Quantitative LC-MS Analysis of Monoclonal Antibodies against Neurodegenerative Disorders**; Jens Rose Fogh[1, 2]; Anne-Marie Jacobsen[1]; Kasper D Rand[2]; Line R. Olsen[1]; *[1]H. Lundbeck A/S, Valby, Denmark; [2]Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark*

TP 647 **Development and Validation of a LC-SRM Method for Simultaneous Quantification of α, β-Tubulin Isotypes in Microtubules from Various Cell Types**; Christine Schaeffer-Reiss[1]; Agnès Hovasse[1]; Alain Van Dorsselaer[1]; Maria M. Magiera[2]; Carsten Janke[2]; Morgane Batzenschlager[3]; Catherine Strassel[3]; François Lanza[3]; *[1]IPHC, UdS, CNRS, UMR7178, Strasbourg, France; [2]Institut Curie, Paris Orsay, France; [3]UMR_S 949 Inserm, EFS-Grand Est, Université de Strasbourg, Strasbourg, France*

TP 648 **Standardizing and Harmonizing Multiple TripleTOF® Systems for DDA and DIA Using a Dedicated Performance Kit**; Nicholas Morrice[1]; Tom Knapman[2]; Hunter Christie[3]; Robert Graham[4]; Julie Brazzatti[4]; Anthony Whetton[4]; *[1]Sciex, Warrington, Cheshire; [2]SCIEX, Warrington, UK; [3]SCIEX, Redwood City, CA; [4]University of Manchester, Manchester, UK*

TP 649 **High Throughput Microflow LC-MS/MS for High Sensitivity Peptide Quantitation in Targeted Assays**; Remco van Soest[1]; Christie Hunter[1]; Morty Razavi[2]; *[1]SCIEX, Redwood City, CA; [2]SISCAPA Assay Technologies, Victoria, BC*

TP 650 **Implementation of Real-Time Update for Time Scheduled Targeted Peptide Quantification (PRM) on a new Quadrupole Orbitrap Benchtop Mass Spectrometer**; Christian Thoeing[1]; Sebastien Gallien[2]; Tabiwang Arrey[1]; Kerstin Strupat[1]; Yue Xuan[1]; Oliver Lange[1]; Markus Kellmann[1]; *[1]Thermo Fisher Scientific, Bremen, Germany; [2]Thermo Fisher Scientific, Courtaboeuf, France*

TP 651 **Towards Comprehensive Signaling Pathway Monitoring Using Advanced PRM Methods**; Sebastien Gallien[1]; Yue Xuan[2]; Shouling Xu[3]; Markus Kellmann[2]; Bhavin Patel[4]; John C. Rogers[4]; Alexander Harder[2]; Andreas F. Huhmer[5]; Ken Miller[5]; *[1]Thermo Fisher Scientific, Courtaboeuf, France; [2]Thermo Fisher Scientific, Bremen, Germany; [3]Carnegie Institution for Science, Stanford, CA; [4]Thermo Fisher Scientific, Rockford, IL; [5]Thermo Fisher Scientific, San Jose, CA*

TP 652 **Endogenous AP-MS to Define the Huwe1 Interactome**; Katelyn Cassidy[1]; Scott A Gerber[1]; *[1]Dartmouth College, Lebanon, NH*

PROTEOMICS: TOP DOWN ANALYSIS II
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TP 653 **Assessment of the Noncovalent Interaction between FGF-2 and Glycosaminoglycans by Chip-Nanoelectrospray High Resolution Mass Spectrometry**; Adrian-Cristian Robu[1]; Laurentiu Popescu[1, 2]; Daniela G. Seidler[3]; Alina D. Zamfir[1]; *[1]National Institute for Research and Development in Electrochemistry and Condensed Matter, Plautius Andronescu Str. 1, RO-300224, Timisoara, Romania; [2]Faculty of Physics, West University of Timisoara, Blvd. Vasile Parvan 4, RO-300223, Timisoara, Romania; [3]Hannover Medical School, Dept. of Gastroentero-, Hepato- and Endocrinology I3, EB2/R3110, Carl-Neuberg-Str. 1, D-30625, Hannover, Germany*

TP 654 **Statistical Fragmentation Pattern Discovery of Intact Proteins Based on their Large-Scale Top-down MS/MS Spectra**; Ruixiang Sun[1, 2]; Ruimin Wang[2]; Hao Chi[2]; Chao Liu[2]; Simin He[2]; Ying Ge[1]; *[1]University of Wisconsin, Madison, WI; [2]Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China*

TP 654 **Statistical Fragmentation Pattern Discovery of Intact Proteins Based on their Large-Scale Top-Down MS/MS Spectra**; Ruixiang Sun[1, 2]; Ruimin Wang[2]; Hao Chi[2]; Chao Liu[2]; Simin He[2]; Ying Ge[1]; *[1]University of Wisconsin, Madison, WI; [2]Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China*

TP 655 **Deciphering the Ubiquitin Code. Top-Down Analysis of Proteins Conjugated with Ubiquitin (Branched Proteins)**; Fabio Gomes[1]; Dapeng Chen[1]; Sitara Chauhan[1]; Dulith Abeykoon[1]; Yan Wang[2]; David Fushman[1]; Catherine Fenselau[1]; *[1]Department of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742; [2]Proteomic Core Facility, University of Maryland, College Park, MD 20742*

TP 656 **Analysis of Myofilament Proteins from Skeletal Muscle Fibers by Top-Down Mass Spectrometry**; Yutong Jin[1]; Ziqing Lin[1]; Gary Diffee[1]; Ying Ge[1]; *[1]University of Wisconsin-Madison, Madison, WI*

TP 657 **Improving High-Throughput Top-Down Proteomics Using a Modified Hybrid Quadrupole-Ultra-High-Field-Orbitrap Mass Spectrometer**; Eugen Damoc[1]; Kyle L. Fort[2]; Michiel van de Waterbeemd[2]; Christian Thoeing[1]; Erik Cousijn[1]; Tabiwang Arrey[1]; Alexander Harder[1]; Albert J. R. Heck[2]; Alexander Makarov[1]; *[1]Thermo Fisher Scientific, Bremen, Germany; [2]Utrecht University, Utrecht, Netherlands*

TP 658 **Coupling Reversed Phase Liquid Chromatography and Capillary Zone Electrophoresis for Top-Down Mass Spectrometry**; Lushuang Huang[1]; Zhe Wang[1]; Hongyan Ma[1]; Si Wu[1]; *[1]University of Oklahoma, Norman, OK*

TP 659 **Mass Measurement Accuracy in Top-Down Protein Identification: Current Limits and Future Prospects**; Christopher L Hendrickson[1, 2]; Lissa C. Anderson[1]; Greg T Blakney[1]; Yuri E Corilo[1]; Lidong He[2]; Tingting Jiang[2]; Alan G. Marshall[1, 2]; Donald F. Smith[1]; Chad R. Weisbrod[1]; *[1]National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; [2]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL*

TP 660 **A Robust Top-down LC/MS-Based Proteomics Platform for Simultaneous Quantification of Protein Expression and Modifications**; Ziqing Lin[1]; Liming Wei[1, 2]; Wenxuan CAI[1]; Wei Guo[3]; Stephen P Ford[3]; Gary M Diffee[1]; Ying Ge[1]; *[1]University of Wisconsin-Madison, Madison, WI; [2]Fudan University, Shanghai, China; [3]University of Wyoming, Laramie, WY*

TP 661 **DRy Ion Localization and Locomotion (DRILL) MS Interface for Sensitivity Enhancement in Top-Down Proteomics**; Alex Jonke[1]; Jung Lee[2]; Peter Kottke[2]; David C. Muddiman[3]; Andrei G Fedorov[2]; Matthew P Torres[1]; *[1]School of Biological Sciences, Georgia Institute of Technology, Atlanta, GA; [2]George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA; [3]Department of Chemistry, North Carolina State University, Raleigh, NC*

TP 662 **Multiplexing FTMS Data Analysis Workflow Improves Downstream Top-Down Structural Characterization of Proteins**; Natalia Gasilova[1]; Konstantin O. Nagornov[2]; Kristina Srzentic[3]; Anton N. Kozhinov[2]; Yury O. Tsybin[2]; Hubert H. Girault[1]; *[1]EPFL Valais, Sion, Valais; [2]Spectroswiss Sàrl, Lausanne, Switzerland; [3]Northwestern University, Evanston, IL*

TP 663 **A User-Friendly Bioinformatics Platform for Automated Continuous Elution Proteoform Analysis**; Casey E Wing[1]; John R Corbett[1, 2]; William S Phipps[1]; Daniel A Plymire[1]; Steven M Patrie[1, 2]; *[1]University of Texas Southwestern Medical Center, Dallas, TX; [2]University of Texas at Dallas, Richardson, TX*

TP 664 **Fixed Charge Chemical Modifications for Enhanced Sequencing of Native-Like Proteins and Protein Complexes**; Daniel Polasky[1]; Philip C Andrews[2, 3]; Brandon T Ruotolo[2]; *[1]University of Michigan, Ann Arbor, MI; [2]University of Michigan, Ann Arbor, MI; [3]University of Michigan Medical School, Ann Arbor, MI*

TP 665 **Charge State Analysis of Native, Denatured, and Carbamylated Proteins by UVPD**; Aarti Bashyal[1]; Sylvester M Greer[1]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

TP 666 **Quantitative Analysis of Free Circulating Light Chains Using a Tribrid Mass Spectrometer and Advanced Bioinformatics**; Moshe Gatt[1]; Alexandra Gabashvili[2]; David Morgenstern[2]; Yishai Levin[3]; *[1]Hadassah Medical Center, Jerusalem, Israel; [2]Weizmann Institute of Science, Rehovot, Rehovot; [3]Weizmann Institute of Science, Rehovot*

TP 667 **Capillary Electrophoresis – Mass Spectrometry for Intact Mass Analysis of Antibodies and Antibody-Drug-Conjugates**; Aran Paulus[1]; Chien-Hsun Chen[2]; Andreas Krupke[3]; Stephane Houel[2]; Daniel Lopez Ferrer[4]; Michael Wenz[3]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, South San Francisco, CA; [4]Thermo Fisher Scientific, San Jose, California*

TP 668 **Autoantibody Biomarker Discovery by Top-Down Proteomics of Serum from Patients with Systemic *Lupus erythematosus***; Zhe Wang[1]; Xiaowen Liu[2]; Kenneth Smith[3]; Si Wu[1]; *[1]University of Oklahoma, Norman, OK; [2]Indiana University-Purdue University Indianapolis, Indianapolis, IN; [3]Oklahoma Medical Research Foundation, Oklahoma City, OK*

TP 669 ***de novo* Sequencing of Proteins by Top-Down 193 nm Ultraviolet Photodissociation Mass Spectrometry**; Kira Vyatkina[1, 2]; Jared B Shaw[3]; Ljiljana Pasa-Tolic[3]; *[1]Saint Petersburg State University, St Petersburg, Russia; [2]SPb Academic University, St Petersburg, Russia; [3]Pacific Northwest National Laboratory, Richland, WA*

TP 670 **Characterization and Quantitation of Tumor-Specific KRAS Proteoforms in Clinical Samples of Colon Cancer by Translational Top-Down Proteomics**; Ioanna Ntai[1]; Luca Fornelli[1]; Josiah Hutton[1]; Ryan T. Fellers[1]; Gordon R. Whiteley[2, 3]; Emily Boja[2, 3]; Henry Rodriguez[2, 3]; Neil L Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]NIH, Bethesda, MD; [3]National Cancer Institute, Bethesda, MD*

TP 671 **Analysis of Intact Hemoglobin Subunits with Ion Parking for Primary Structure Characterization**; Elizabeth Duselis[1]; Jane Yang[2]; Scott Ugrin[1]; Dina L Bai[1]; Jeffrey Shabanowitz[1]; David Herold[2]; Donald F. Hunt[1]; *[1]University of Virginia, Charlottesville, VA; [2]University of California, San Diego, La Jolla, CA*

TP 672 **MASH Explorer, a Universal Software Environment for Top-Down Proteomics**; Zhijie Wu[1]; Sean McIlwain[1]; Wenxuan Cai[1]; Huseyin Guner[1]; Irene M. Ong[1]; Yiwen Gu[1]; Sudharshanan Govindaraj Ramanathan[1]; Xiaowen Liu[2]; Ruixiang Sun[3]; Ying Ge[1]; *[1]University of Wisconsin-Madison, Madison, WI; [2]Indiana University−Purdue University Indianapolis, Indianapolis, IN; [3]Chinese Academy of Science, BeiJing, China*

TP 673 **Comparative Label-Free Quantitation of Mouse Brain Tissue Proteoforms Using Top-Down Proteomics**; Hae-Min Park[1]; Roderick G. Davis[1]; Ryan T. Fellers[1]; Joseph B. Greer[1]; Elena V. Romanova[2]; Stanislav S. Rubakhin[2]; Richard D. LeDuc[1]; Paul M. Thomas[1]; Justin S. Rhodes[2]; Jonathan V. Sweedler[2]; Neil L Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]University of Illinois at Urbana-Champaign, Urbana, IL*

TP 674 **Expanding Proteoform Identifications by Constructing Proteoform Families from Intact-Mass Measurements in Top-Down Proteomic Data**; Leah V. Schaffer[1]; Michael R. Shortreed[1]; Anthony J. Cesnik[1]; Brian L. Frey[1]; Stefan K. Solntsev[1]; Mark Scalf[1]; Lloyd M. Smith[1]; *[1]University of Wisconsin Madison, Madison, WI*

TP 675 **Proteoform Dynamics**; Tao Wang[1]; Mathew V. Holt[1]; Nicolas Leon Young[1]; *[1]Baylor College of Medicine, Houston, TX*

TP 676 **Validation of Chagas' Disease Serum Biomarkers by Intact Proteins Analysis**; Elizabeth Ruiz Lancheros[1]; Pierre-Olivier Schmit[2]; Eric Chatelain[3]; Jaime Altcheh[4]; Momar Ndao[1]; *[1]Research Institute - McGill University Health Centre, Montreal, Qc; [2]Bruker Daltonics, Strasbourg, France; [3]Drugs for Neglected Diseases initiative (DNDi), Geneva, Switzerland; [4]Hospital de Niños Dr. Ricardo Gutierrez, Buenos Aires, Argentina*

TP 677 **In-Depth Characterization of Intact Protein Standards Using HRAM Top Down Mass Spectrometry with Multiple MSMS Strategies**; Romain Huguet[1]; Helene Cardasis[1]; Christopher Mullen[1]; Stephane Houel[1]; Luca Forneli[2]; Rosa Viner[1]; Viktorija Vitkovskė[3]; Shanhua L. Lin[4]; Seema Sharma[1]; Vlad Zabrouskov[1]; Neil L. Kelleher[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Northwestern University-Kelleher Research Group, Evanston, IL; [3]Thermo Fisher Scientific, Vilnius, LT; [4]Thermo Fisher Scientific, Sunnyvale, CA*

TP 678 **Quantitative, Localized Analysis of Mouse Brain Subregions by Top-Down Proteomics**; Roderick G. Davis[1]; Hae-Min Park[2]; Paul M. Thomas[2]; Ryan T. Fellers[2]; Joseph B. Greer[2]; Richard D. LeDuc[2]; Amy W. Lasek[3]; Rosalba Satta[3]; Jonathan V Sweedler[4]; Evena V. Romanova[4]; Stanislav Rubakhin[4]; Neil L. Kelleher[2]; *[1]Northwestern University, Evanston, IL; [2]Northwestern University, Evanston, IL; [3]University of Illinois at Chicago, Chicago, IL; [4]University of Illinois at Urbana-Champaign, Urbana, IL*

TP 679 **Top-Down Proteomic Analysis with Capillary Zone Electrophoresis-Mass Spectrometry**; Robert N. O'meally[1]; Simion Kreimer[1]; Robert N. Cole[1]; *[1]Mass Spectrometry and Proteomics Facility, Johns Hopkins School of Medicine, Baltimore, MD*

SMALL MOLECULES: QUALITATIVE ANALYSIS
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TP 680 **Elimination of Toluene during Collision-Induced Fragmentation of Deprotonated N,N'-Diphenylacetyldapsone Generated by Negative-Ion Electrospray Ionization Mass Spectrometry**; Chongming Liu[1]; Athula Attygalle[1]; *[1]Stevens Institute of Technology, Hoboken, NJ*

TP 681 **Targeted Determination of Lipid Mediators in Mice Muscle Tissues Using Restricted Access Media-Based Pretreatment and Liquid Chromatography-Mass Spectrometry**; Zhiying Wang[1]; Liangqiao Bian[2]; Chenglin Mo[1]; Maciej Kukula[3]; Kevin A. Schug[4]; Marco Brotto[1]; *[1]College of Nursing and Health Innovation, The University of Texas at Arlington,, Arlington, TX 76019; [2]SCAAC, University of Texas at Arlington, Arlington, TX 76019; [3]SCAAC, UT Arlington, Arlington, TX 76019; [4]Departments of chemistry and biochemistry, UT Arlington, Arlington, TX*

TP 682 **Quantitative Measurement of Unconjugated Phenylephrine in Human Plasma via UHPLC with Tandem Mass Spectrometry**; Jingduan Chi[1]; Yonghua Ling[1]; Rand Jenkins[2]; Fumin Li[1]; *[1]PPD Inc, Madison, WI; [2]PPD Inc, Richmond, VA*

TP 683 **Challenges Developing Sensitive Quantitative Assaysfor Cyclophosphamide and 4-Hydroxycyclophosphamide in Human Plasma Using HPLC-MS/MS**; Aihua Liu[1]; Lijuan Fu[1]; Qian Guo[1]; Bryce Ashby[1]; Scott Reuschel[1]; Min Meng[1]; *[1]Covance, Salt Lake City, UT*

TP 684 **Development and Validation of an LC-MS/MS Method for the Quantitation of Plerixafor in Human Plasma and Urine**; Hui Hong[1]; Dawei Zhou[2]; Baomin Xin[1]; Xinping Fang[2]; Xin Zhang[1]; *[1]WuXi AppTec (Shanghai) Co. Ltd, Shanghai, China; [2]WuXi AppTec. Inc, Plainsboro Township, NJ*

TP 685 **Elimination of Endogenous Light-Sensitive Compounds in Human Plasma by UV-Irradiation for the Determination of Tretinoin and Isotretinoin by LC-MS/MS**; Romain Beauvois[1]; Milton Furtado[1]; Anahita Keyhani[1]; *[1]Altasciences, Laval, QC*

TP 686 **Identification Criteria for the Analysis of Biomarkers of Chemical Warfare Agents**; R.V.S. Murty Mamidanna; *Organisation for the Prohibition of Chemical Weapons, The Hague, Netherlands*

TP 687 **Elimination of Ionization Suppressing Dosing Excipient from LC-MS Method for Bendamustine and M3 in Human Plasma**; Theodore Brus; *Covance, Indianapolis, IN*

TP 688 **Quantitation of Lidocaine and Its Metabolites in Human Plasma**; Adrian Bott[1]; Tim Shoaf[2]; *[1]BASi, West Lafayette, IN; [2]BASi, West Lafayette, IN*

TP 689 **Analysis of Extractable and Leachable (E&L) Compounds Using a Novel Low-Energy EI Capable High Resolution Accurate Mass GC/Q-TOF**; Kevin Rowland[1]; Mark Jordi[1]; Kai Chen[2]; Jennifer Sanderson[2]; *[1]Jordi Labs, Mansfield, MA; [2]Agilent Technologies, Santa Clara, CA*

TP 690 **Extractable Study of a Drug Delivery Device - Vaginal Rings**; Li Xu[1]; John Iannone[1]; Wei Zhang[1]; Kate Comstock[2]; Ekong Bassey[3]; John Schmelzel[3]; Tom Carrell[3]; *[1]AMRI, Albany, NY; [2]Thermo Fisher Scientific, San Jose , CA; [3]Thermo Fisher Scientific, San Jose, CA*

TP 691 **Extractables Analysis of Pharmaceutical Container/Packaging Labels**; John Iannone[1]; Li Xu[1]; Wei Zhang[1]; Kate Comstock[2]; Ekong Bassey[3]; John Schmelzel[4]; Tom Carrell[4]; *[1]AMRI, Albany, NY; [2]Thermo Fisher Scientific, San Jose , CA; [3]ThermoFisher, San Jose, CA; [4]Thermo Fisher Scientific, San Jose, CA*

TP 692 **Fragmentation Patterns in the Mass Spectra of Fentanyl-Type Compounds**; Kirill Tretyakov[1]; Edward White V[1]; Stephen Stein[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

TP 693 **LC/MS/MS Method Validation for the Determination of Methamphetamine Enantiomers in Human Urine Utilizing a Novel Production Friendly Chiral Column**; Amber Awad[1]; Ana Celia Grenier Ph.D[1]; Lawrence J. Andrade[1]; *[1]Dominion Diagnostics, North Kingstown, RI*

TP 694 **Development and Validation of a Simple & Rugged LC-MS/MS Method for Determination of Unbound and Total Tiopronin in Human Plasma**; Ben Gaboury[1]; Nick Peng[1]; Ardeshir Khadang[1]; *[1]Axis Clinicals, Dilworth, MN*

TP 695 **Development and Validation of a Sensitive and Rugged LC-MS/MS Method to Measure Phenylephrine and Chlorpheniramine in Human Plasma**; Nick Peng[1]; Ben Gaboury[1]; Ardeshir Khadang[1]; *[1]Axis Clinicals, Dilworth, MN*

TP 696 **Non-Targeted Characterization of Low Molecular Weight Organic Matter along Alaskan Soil Depth Profile Using RP and HILIC Coupled with nano-ESI-HRMS/MS**; Mallory P Ladd[1]; Colleen M Iversen[1, 2]; Stan D Wullschleger[2, 3]; Shawn R Campagna[4]; Robert L Hettich[1, 5]; *[1]Bredesen Center for Interdisciplinary Research and Graduate Education, Knoxville, TN; [2]Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN; [3]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN; [4]Department of Chemistry, University of Tennessee, Knoxville, TN; [5]Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN*

TP 697 **Stability Evaluation of Captopril in Human Blood by LC-MS/MS**; Eugenie Raphaelle Bérubé[1]; Milton Furtado[1]; Anahita Keyhani[1]; *[1]Altasciences, Laval , QC*

TP 698 **An LC-MS Screening Platform to Simultaneously Detect Clinically Relevant Antibiotics in Cholera Patient Urine and Stool**; Ludmila Alexandrova[1]; Allis Chien[1]; Vasavi Ramachandran[2]; Paul Bollyky[3]; Eric Nelson[2, 4]; *[1]Stanford University Mass spectrometry, Stanford, CA; [2]Department of Pediatrics, Stanford, CA; [3]Department of Medicine, Stanford, CA; [4]Emerging Pathogens Institute, Department of Pediatrics, University of Florida, Gainesville, FL*

TP 699 **Characterization of Industrial Amine-Based UVC Products by Chromatography-Mass Spectrometry (GC/GCMS, LC/LCMS) for REACH Registration**; Dale A. Willcox[1]; Steve E. Deppen[1]; Kelli L. Magarelli[1]; Noelle M. Elliott[1]; *[1]Intertek Allentown, Allentown, PA*

TP 700 **Towards Quantitative Analysis without Standards: Chromatographic Retention Time as a Predictor of Mass Spectrometric Response Factor**; Daniel Foil[1]; Nadja B. Cech[1]; Daniel A Todd[1]; *[1]University of North Carolina at Greensboro, Greensboro, NC*

TP 701 **Multi-Class, High-Throughput Analysis of Drugs in Equine Urine and Blood by Liquid Chromatography-High Resolution Accurate Mass Spectrometry for Racing Regulation**; Efthimia Papastavros[1]; Kenneth P. Matuszak[2]; David J. Borts[1]; *[1]Iowa State University, Ames, Iowa; [2]Thermo Fisher Scientific, Bannockburn, IL*

TP 702 **Spatially Resolved, Quantitative Analysis of Small Molecules in Tissue Using A Laser Capture Microdissection (LCM)-LC/MS Platform**; Chenqi Hu[1]; Jamie Erickson[2]; Youngjae Kim[2]; Soumya Mitra[2]; Stephanie Gaudette[2]; Annette Schwartz Sterman[2]; David Duignan[2]; Edit Tarcsa[2]; *[1]AbbVie, Worcester, MA; [2]AbbVie, Worcester, MA*

TP 703 **UVPD as a Unique Fragmentation Tool for Complete Structure Determination and Substructure Identification of Small Molecules**; Romain Huguet[1]; Seema Sharma[1]; Christopher Mullen[1]; Jesse Canterbury[1]; Mark Berhow[2]; Vlad Zabrouskov[1]; Tim J. Stratton[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]USDA, ARS, NCAUR, Peoria, IL*

TP 704 **Generation of an Electronic Cigarette Liquid Profile Library Using GCQTOFMS and Chromatographic Deconvolution and Comparison Software to Screen for Additives**; Hayley Abbiss[1, 2, 3]; John H Moncur[1]; Scott J Campbell[1]; Robert D Trengove[2, 3]; *[1]SpectralWorks, Runcorn, UK; [2]Murdoch University, Perth, Western Australia; [3]Separation Science and Metabolomics Laboratory, Murdoch University, Perth, Australia*

TP 705 **A Comparison of the Reactivity of Para-Benzynes in Gas Phase and Solution**; Rashmi Kumar[1]; Hilkka Kenttamaa[2]; *[1]Purdue University, West Lafayette, Indiana; [2]Purdue University-Department of Chemistry, West Lafayette, IN*

SMALL MOLECULES: QUANTITATIVE ANALYSIS II
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TP 706 **Long-Term Monitoring of di-(2-Ethylhexyl)Phthalate (DEHP) Exposure in Hair Using On Line Solid Phase Extraction and Liquid Chromatography Tandem Mass Spectrometry**; Yan Zin Chang; *, Taichung, Taiwan*

TP 707 **An LC-MS/MS Method Improvement and Validation for Determination of Yeliva in Rat and Dog Plasma**; Xiaodong Shen[1]; Xiao Ming Gan[1]; Rwaida Al-Eryani[1]; Sridhar Korasikha[1]; Sangeeta Rajasingam[1]; Alain Guimond[2]; Reza Fathi[3]; Gary Johnson[1]; *[1]ITR Laboratories, Montreal, QC; [2]Insymbiosis, Montreal, Qc; [3]RedHill Biopharm Ltd., Tel Aviv, Israel*

TP 708 **Simultaneous Determination of Sugar Phosphates in Cancer Cells by Capillary Electrophoresis-Mass Spectrometry**; Miso Nam[1, 2]; Sunhee Jung[1, 2]; Do Hyun Ryu[1]; Geum-Sook Hwang[2]; *[1]Sungkyunkwan University, Suwon, South Korea; [2]Korea Basic Science Institute, Seoul, South Korea*

TP 709 **Versatile Strategies for Analysis of Sulfonate Ester Related Genotoxic Impurities Based on High Performance Chromatography Combined with Mass Spectrometry**; Zheng-Xiang Zhang[1]; TAO BO[1]; *[1]Agilent Technologies (China), Beijing*

TP 710 **Rapid Analysis of Histidine, Anserine and Carnosine in Mouse Skeletal Muscle Tissue by HILIC UPLC-MS/MS**; David Hoetker[1, 2]; Adjoa Boakye[1, 2]; Jaron Thomas[1, 2]; Jingjing Zhao[1, 2]; Shahid Baba[1, 2]; *[1]University of Louisville, Louisville, KY; [2]Diabetes and Obesity Center, U of L, Louisville, KY*

TP 711 **Determination of Fluticasone Propionate, Salmeterol, Naltrexone, and Buprenorphine in Human Plasma with Ultra-Sensitive LC-MS/MS Methods**; Dawei Zhou[1]; Pei Li[1]; Thomas moran[2]; Mohamed Osman[1]; Xinping Fang[1]; *[1]WuXi AppTec, Plainsboro, NJ; [2]Shimadzu Scientific Instruments, Somerset, NJ*

TP 712 **An Ultrafast LC/MS/MS Method for Characterization and Quantitation of Triton X-100 Extracted from Palm Oil**; Udi Jumhawan[1]; Jie Xing[1]; Zhaoqi Zhan[1]; *[1]Shimadzu Asia Pacific, Singapore, Singapore*

TP 713 **Quantitation of Endogenous β-Hydroxy-β-Methylbutyric Acid in Human Blood: Comparison between Dried Blood Spot, Dried Plasma Spot, and Liquid Plasma Analysis**; Carl Noren[1]; Stefan Ehling[1]; Todime Reddy[1]; *[1]Abbott Nutrition, Columbus, OH*

TP 714 **Validated LC-MS/MS Assay for Quantitation of Paclitaxel in Human Seminal Fluid**; Robert Clegg[1]; Rachel Sun[2]; *[1]BASi, West Lafayette, IN; [2]BASi, West Lafayette, IN*

TP 715 **Sensitive Quantitative Measurement of Cortisol from Limited Human Hair Samples Using LC-MS/MS**; David W. Erikson[1]; Amy V. Kaucher[1]; Emily Agan[1]; Andrea J. Winchell[1]; Steven W. Blue[1]; Ashley Scherman[2]; Cynthia T. McEvoy[2]; Eliot R. Spindel[1]; *[1]Oregon National Primate Research Center, Beaverton, OR; [2]Oregon Health & Science University, Portland, OR*

TP 716 **An LC-MS/MS Method to Detect Antibiotic Residues in Distillers Grains to Address Concerns of Potential Antimicrobial Resistance Development**; Hemakanthi De Alwis[1]; Kaleb J Duelge[1]; Upul Nishshanka[1]; *[1]Office of Research, Center for Veterinary Medicine, Food and Drug Administration, Laurel, MD*

TP 717 **A Rugged Bioanalytical Method for Quantification of Liraglutide in Human Plasma by LC-MS-MS**; Karin Keller[1]; Heather McLaughlin[1]; Laura Binneboese[1]; Edward Wells[1]; Steve Unger[1]; *[1]Worldwide Clinical Trials, Austin, TX*

TP 718 **Method Development and Validation for the Quantification of Fulvestrant in Human Plasma Using LC-MS/MS**; Guodong Gu[1]; Yinghe Li[1]; Anna Fiorella[1]; Colt Cookson[1]; *[1]Alliance Pharma, Malvern, PA*

TP 719 **Screening Method for Methamphetamine and Amphetamine Using DART® MS Analysis Followed by Chiral Confirmation for D-Methamphetamine**; Craig Aurand[1]; Candace Price[1]; Sara Smith[1]; Emily Barrey[1]; *[1]MilliporeSigma, Bellefonte, PA*

TP 720 **Analytical Data Longevity and Management for Regulatory Compliance Using AnIML Format and Cloud Technologies**; John Gibbons[1]; Viktor N Iassinskii[2]; Burkhard Schaefer[3]; *[1]SCIEX, Concord, ON; [2]Sciex, Concord, ON; [3]BSSN Software GmbH, Darmstadt, Germany*

TP 721 **Trimester-Specific Progesterone Reference Intervals Established in Human Serum/Plasma Using a Fast LC-MS/MS Method Coupled with Differential Ion Mobility Spectrometry**; Julie A Ray[1]; Joely A Straseski[1, 2]; *[1]ARUP Laboratories, Salt Lake City, UT; [2]University of Utah, Salt Lake City, UT*

TP 722 **Implementing GMP Impurity Methods on a Single Quadrupole LC/MS**; Laura Hayter[1]; Philip Anderson[1]; Madelyn Hunsley[1]; *[1]Avista Pharma Solutions, Longmont, CO*

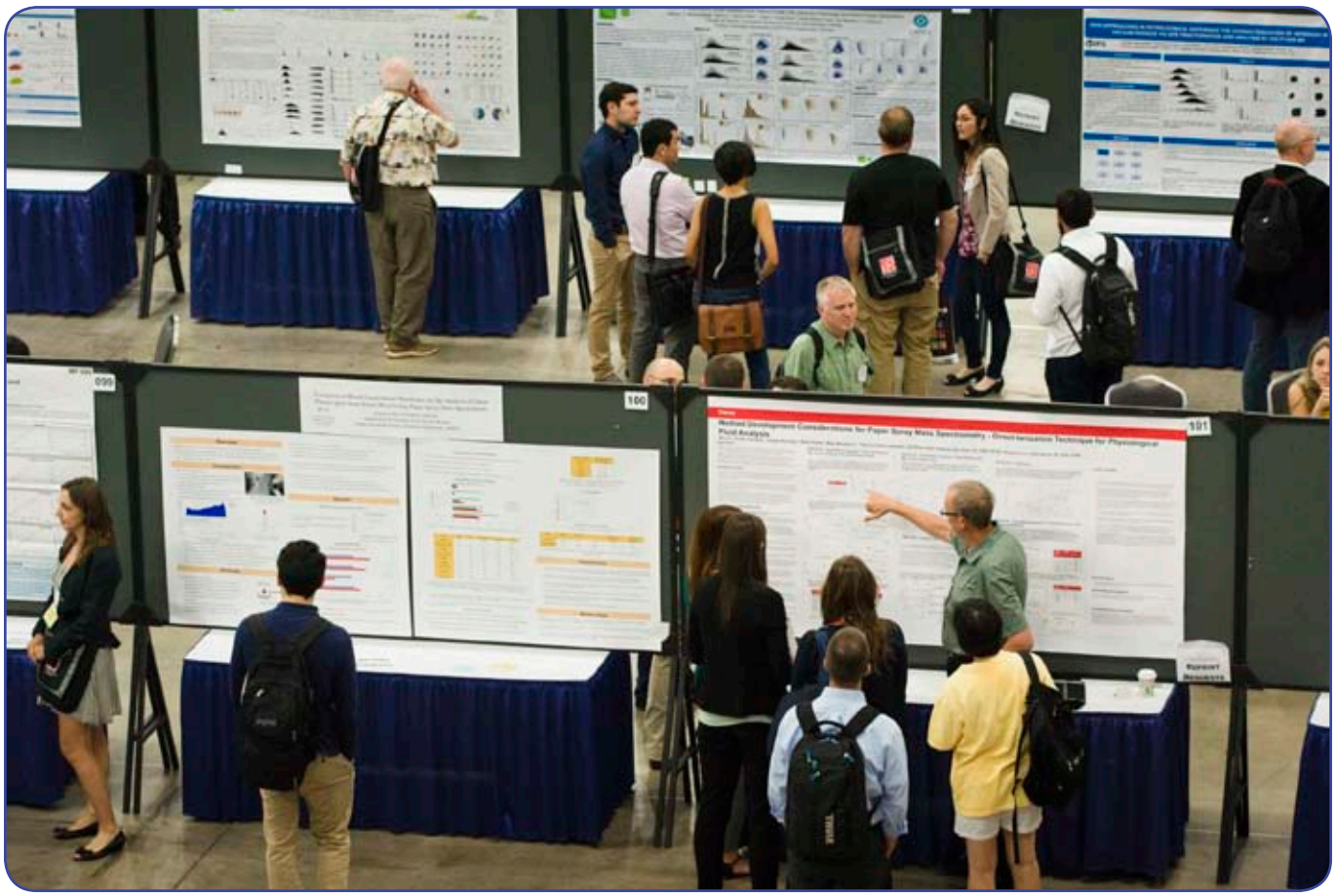
TP 723 **Chiral Derivatization of D- and L-Eflornithine for Enantiomer Identification from a Racemate and Chromatographic Separation**; Abram Brubaker[1]; Neal Simmons[1]; Ashley Brant[1]; Ronald Shoup[1]; *[1]AIT Bioscience, Indianapolis, IN*

TP 724 **Development of LC-MS/MS Detection Strategies in Rapamycin and Seco-rapamycin Whole Blood Bioanalysis**; Tobias Magers[1]; Brian Engel[1]; Abram Brubaker[1]; Brad King[1]; Ashley Brant[1]; Ronald Shoup[1]; *[1]AIT Bioscience, Indianapolis, IN*

TP 725 **A Rugged, Robust, Stereo-Selective LC/MS/MS Method for Simultaneous Determination of Two Enantiomers of a Small Molecule Antibiotic in Human Plasma**; Ze Li[1]; Patricia A. Hansen[1]; Maral Llewellyn[1]; *[1]Covance, Indianapolis, IN*

TP 726 **Analysis of Anamorelin Stereoisomers in Human Plasma Using Coupled Achiral / Chiral HPLC with Tandem Mass Spectroscopy Detection**; Steven X. Yan[1]; Anika Pippin[1]; Yu-Hui Ann Fu[1]; Julie Showalter[1]; Gene Ray[1]; Alberto Bernareggi[2]; Elizabeth Duus[3]; Yansheng Liu[1]; *[1]KCAS Bioanalytical Services, Shawnee, KS; [2]Helsinn Healthcare SA, Lugano, Switzerland; [3]Helsinn Therapeutics (US), Inc., Iselin, NJ*

TP 727 **A High Sensitivity LC/MS/MS Method for Quantitative Analysis of Five Carcinogenic Dyes in Textiles**; Yin Ling Chew[1]; Felicia Xue Qi Tan[2]; Yi Hao Wee[3]; Jarren Ling Yao Tuang[2]; Djohan Kesuma[1]; Jie Xing[1]; Zhaoqi Zhan[1]; *[1]Shimadzu Asia Pacific, Singapore; [2]School of Physical and Mathematical Science, Nanyang Technical University, Singapore; [3]National University of Singapore*



AMBIENT IONIZATION: APPLICATIONS II
001 - 034

WP 001 **Spontaneous Desalting Droplet Spray Ionization for Direct and Sensitive Analysis of Seawater Sample**; Hong Zhang[1]; Jing He[2]; Na Li[2]; Jie Jiang[2]; *[1]State Key Laboratory of Urban Water Resource and Environment, Harbin Institute of Technology, Harbin, China; [2]School of Marine Science and Technology, Harbin Institute of Technology at Weihai, Weihai, China*

WP 002 **Development of an In Vivo Real-time Monitoring System using Probe Electrospray Ionization/ Tandem Mass Spectrometry (PESI/MS/MS) and its Preliminary Applications**; Kei Zaitsu[1, 2]; Yumi Hayashi[1, 3]; Tasuku Murata[4]; Tomomi Ohara[2]; Stéphane Moreau[5]; Maiko Kusano[2]; Hiroki Nakajima[6]; Hiroshi Tanihata[4]; Hitoshi Tshuchihashi[2]; Tetsuya Ishikawa[3]; Akira Ishii[2]; *[1]In Vivo Real-Time Omics Laboratory, Institute for Advanced Research, Nagoya University, Nagoya, Japan; [2]Department of Legal Medicine and Bioethics, Nagoya University Graduate School of Medicine, Nagoya, Japan; [3]Pathophysiological Laboratory Sciences, Department of Radiological and Medical Laboratory Sciences, Nagoya University Graduate School of Medicine, Nagoya, Japan; [4]Shimadzu Corporation, Kyoto, Japan; [5]Shimadzu Europe GmbH, Duisburg, Germany; [6]European Innovation Center, Shimadzu Europa GmbH, Duisburg, Germany*

WP 003 **High-throughput Intact Metabolome Analysis of Mouse Biological Specimens by Probe Electrospray Ionization/Tandem Mass Spectrometry (PESI/MS/MS)**; Yumi Hayashi[1, 2]; Kei Zaitsu[1, 3]; Tasuku Murata[4]; Shiono Baba[3]; Tomomi Ohara[3]; Stéphane Moreau[5]; Maiko Kusano[3]; Hiroki Nakajima[6]; Hiroshi Tanihata[4]; Hitoshi Tsuchihashi[3]; Akira Ishii[3]; Tetsuya Ishikawa[2]; *[1]In Vivo Real-Time Omics Laboratory, Institute for Advanced Research, Nagoya University, Nagoya, Japan; [2]Pathophysiological Laboratory Sciences, Department of Radiological and Medical Laboratory Sciences, Nagoya University Graduate School of Medicine, Nagoya, Japan; [3]Department of Legal Medicine and Bioethics, Nagoya University Graduate School of Medicine, Nagoya, Japan; [4]Shimadzu Corporation, Kyoto, Japan; [5]Shimadzu Europa GmbH, Duisburg, Germany; [6]European Innovation Center, Shimadzu Europa GmbH, Duisburg, Germany*

WP 004 **Combining Molecularly Imprinted Polymer (MIP) and Paper Spray Mass Spectrometry for Agrochemical Screening in Foodstuffs**; Boniek Gontijo Vaz[1]; Igor Pereira[1]; Andréia Rodrigues Chaves[1]; *[1]Federal University of Goiás, Goiânia, GO*

WP 005 **Coupling PaperSpray Technology to High-End Orbitrap Mass Spectrometry**; Kerry Hassell[1]; Maria C. Prieto Conaway[2]; *[1]ThermoFisher Scientific, Somerset, NJ; [2]ThermoFisher Scientific, San Jose, CA*

WP 006 **Depth-resolved Metabolite Analysis on a Plant Surface by Nanospray Desorption Electrospray Ionization (nano-DESI) Mass Spectrometry**; Sangwon Cha[1]; Gyuwoong Jun[1]; Dongkun Lee[1]; Purum Kim[1]; *[1]Hankuk University of Foreign Studies, Yongin, South Korea*

WP 007 **Illumination-assisted Droplet Spray Ionization: In Situ Analysis and Real-time Monitoring of Photocatalytic Reactions**; Jie Jiang[1]; Hong Zhang[2]; Na Li[1]; *[1]School of Marine Science and Technology, Harbin Institute of Technology at Weihai, Weihai, China; [2]State Key Laboratory of Urban Water Resource and Environment, Harbin Institute of Technology, Harbin, China*

WP 008 **Improving Quantification using PaperSpray Ionization Coupled to Ion Trap Mass Spectrometry for Clinical Research**; Cornelia Leonie Boeser[1]; Linfan Li[1]; Jae C. Schwartz[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

WP 009 **Investigating the Structural Transitions of Proteins during Dissolution by Mass Spectrometry**; Xiaoyun Gong[1]; Xingchuang Xiong[2]; Xiang Fang[2]; *[1], Beijing, Beijing; [2]National Insititute of Metrology, Beijing, China*

WP 010 **Molecular Discrimination of Follicular Thyroid Adenomas and Carcinomas using Ambient Ionization Mass Spectrometry**; Rachel J. DeHoog[1]; Jialing Zhang[1]; Elizabeth Alore[2]; Wendong Yu[2]; Rob Tibshirani[3]; Anton F Engelsman[4, 5]; Stan B Sidhu[4, 5]; James Suliburk[2]; Livia S. Eberlin[1]; *[1]University of Texas at Austin, Austin, TX; [2]Baylor College of Medicine, Houston, TX; [3]Stanford University, Stanford, California; [4]Royal North Shore Hospital, Sydney, Australia; [5]University of Sydney, Sydney, Australia*

WP 011 **Online Examination of Catalytic Oxidation of Glucose by Ambient Liquid-Assisted Ionization Mass Spectrometry**; Yan Wang[1]; Jin Ouyang[1]; Na Na[1]; *[1]Beijing Normal University, Beijing, China*

WP 012 **Picomole-Scale Real-Time Photoreaction Screening: Discovery of the Visible-Light-Promoted Dehydrogenation of Tetrahydroquinolines under Ambient Conditions**; Qiongqiong Wan[1]; Suming Chen[2];

Abraham K. Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH; [2]Johns Hopkins University, Baltimore, MD*

WP 013 **Preparative Electrospray and Preparative Reactive Extractive Electrospray for Route Prediction and Optimization of Atropine Synthesis in Microfluidics**; Caitlin Falcone[1]; Zinia Jaman[1]; Michael Wleklinski[1]; Andy Koswara[1]; David H. Thompson[1]; R. Graham Cooks[1]; *[1]Purdue University, West lafayette, IN*

WP 014 **The Utility of Hydrophobic Paper Strips in the Direct Analysis of Dried Biofluids Using Mass Spectrometry**; Deidre E. Damon[1]; Abraham K. Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

WP 015 **Thread Spray Mass Spectrometry for In-Situ Analysis of Capsaicinoids**; Sierra Jackson[1]; Devin J. Swiner[1]; Bridget K. Walsh[1]; Yaman Kouatli[1]; Abraham K. Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

WP 016 **Whole Body Skin Imagings of Medicines and Metabolitesby Thermal Desorption-Electrospray Ionization/Mass Spectrometry**; Jentaie Shiea [1]; Jia-Ming Lin[1]; Yang-Kuang Pan[1]; Yu-Hsuan Kuo[1]; Hung Su[1]; *[1]National Sun Yat-Sen University, Kaohsiung, Taiwan*

WP 017 **Acceleration of Claisen-Schmidt Reaction with Preparative Sonic Spray Ionization**; Zhenwei Wei[1]; Michael Wleklinski[1]; Caitlin E. Falcone[1]; Graham Cooks[1]; *[1]Purdue University, West lafayette, IN*

WP 018 **Amino Acids Desalt Protein Samples during DESI-MS Analysis**; Roshan Javanshad[1]; Elahe Honarvar[1]; Andre R. Venter[1]; *[1]Western Michigan University, Kalamazoo, MI*

WP 019 **Application of T-probe to MS Metabolomics analysis of live single cells**; Renmeng Liu[1]; Yanlin Zhu[1]; Ning Pan[1]; Zhibo Yang[1]; *[1]University of Oklahoma, Norman, OK*

WP 020 **Automated PaperSpray Sample Preparation using a Robotic Autosampler for Clinical Research**; Steven L. Reeber[1]; Lucas Luethy[2]; Cornelia Leonie Boeser[1]; John Glazier[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]CTC Analytics AG, Zwingen, Switzerland*

WP 021 **Detection and Imaging of Thermochromic Ink Compounds in Erasable Pens using Desorption Electrospray Ionization Mass Spectrometry (DESI-MS)**; Amin Khatami[1]; Shamina Prova S. Prova[1]; Aafreen Bagga[1]; Michelle Ting[1]; Gurnoor Brar[1]; Demian R. Ifa[1]; *[1]York University, Toronto, ON, Canada*

WP 022 **Distinguishing Non-Small Cell Lung Cancer Subtypes by Desorption Electrospray Ionization Mass Spectrometry**; Alena Bensussan[1]; Tanweer Zaidi[2]; Ruth Katz[2]; Erik Cressman[2]; LIVIA S. EBERLIN[1]; *[1]University of Texas at Austin, Austin, TX; [2]MD Anderson Cancer Center, Houston, TX*

WP 023 **Evaluation of Stainless Steel Electrospray Electrodes in Micro LC-MS/MS Analysis**; Tomasz Bienkowski[1, 2]; Konrad Piotr Kowalski[1, 2]; *[1]MS Ekspert Sp. z o.o., Gdańsk, Poland; [2]Masdiag Sp. z o.o., Warszawa, Mazowieckie*

WP 024 **Metabolite, Lipid, and Peptide Analysis of Single Neurons of Known Function in Lymnaea stagnalis by Capillary Microsampling Mass Spectrometry**; Linwen Zhang[1]; Nikkita Khattar[1]; Zita Zrinyi[2]; Zsolt Pirger[2]; Ildiko Kemenes[3]; Gyorgy Kemenes[3]; Akos Vertes[1]; *[1]The George Washington University, Washington, DC; [2]Balaton Limnological Institute, Tihany, Hungary; [3]University of Sussex, Brighton, UK*

WP 025 **Methodologies for Investigating Neurodegenerative Disorders using a Liquid-Microjunction Surface Sampling Probe**; Emily L. Gill[1]; Megan Marks[1]; Richard A. Yost[1]; Vinata Vedam-Mai[1]; Timothy J. Garrett[1]; *[1]University of Florida, Gainesville, FL*

WP 026 **Negative Ion Paper Spray for the Detection of Acidic Compounds**; Josiah McKenna[1]; Trevor Glaros[2]; Nicholas E. Manicke[1]; *[1]Indiana University−Purdue University Indianapolis, Indianapolis, IN; [2]US Army ECBC, Aberdeen Proving Ground, MD*

WP 027 **Paper Spray High-Resolution Accurate-Mass Spectrometry for Rapid Quantitation of NSAID Drugs in Equine Plasma**; David J. Borts[1]; Joseph H. Kennedy[2]; *[1]Iowa State University, Ames, IA; [2]Prosolia, Inc., Indianapolis , IN*

WP 028 **Predictive Models of Negative Ion Electrospray Response Explored through Machine Learning Applications**; Melanie T. Odenkirk[1]; Ren T. Blackart[1]; James M. Matilla[1]; Michael L. Poltash[1]; Stephen K. Lucas[1]; Christine A. Hughey[2]; Jeff Jones[3]; *[1]James Madison University, Harrisonburg , VA; [2]James Madison University, Harrisonburg , VA; [3]SoCal Bioinformatics Inc., Glendale, CA*

WP 029 **Rapid Analysis of Forensic Related Samples using Ambient Ionization Techniques Coupled to High Resolution Mass Spectrometers**; Eshwar Jagerdeo[1]; Amanda Wriston[2]; *[1]FBI Laboratory, Quantico, VA; [2]FBI Laboratory, Huntsville, AL*

WP 030 **Reaction Screening using Accelerated Reactions in Leidenfrost Droplets**; Kiran Iyer[1]; H. Samuel Ewan[2]; Seok-Hee Hyun[2]; Michael Wleklinski[2]; David H. Thompson[2]; R.Graham Cooks[2]; *[1]Purdue University, West Lafayette, IN; [2]Purdue University, West lafayette, IN*

WP 031 **Direct Analysis of Alloys by Electrochemistry Spray Ionization Mass Spectrometry**; Jiaquan Xu[1]; Tenggao Zhu[1]; Runhan Yan[1]; Huanwen Chen[1]; *[1]East China University of Technology, Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, Nanchang, China*

WP 032 **MS Chemical Fingerprints Reveal the Molecular Dependence of Exhaust Particulate Matters on the Engine Speed**; Yi Li[1]; Hua Zhang[1]; Kun Liu[1]; Feifan Jie[1]; Liang Zhu[1]; Huanwen Chen[1]; *[1]East China University of Technology, Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, Nanchang, China*

WP 033 **Rapid Identification of Meat Species by Internal Extractive Electrospray Ionization Mass Spectrometry of Hemoglobin Selectively Extracted on Functionalized Graphene Oxide**; Lili Song[1]; Jiaquan Xu[1]; Konstantin Chingin[1]; Huanwen Chen[1]; *[1]East China University of Technology, Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, Nanchang, China*

WP 034 **Investigation on the Dehydroxylation of Hydroxyl Polycyclic Aromatic Hydrocarbons by Ambient Mass Spectrometry**; Xiaoping Zhang[1]; Yi Li[1]; Jiaquan Xu[1]; Huanwen Chen[1]; *[1]East China University of Technology, Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, Nanchang, China*

BIOMARKERS: QUANTITATIVE ANALYSIS II
035 - 064

WP 035 **High-thought Determination of Tryptophan and KynurenineinIDO Assay by LC-MS/MS**; Xinfa Fu[1]; Hongmei Wang[1]; YI TAO[1]; Xinping Fang[1]; Xin Zhang[1]; *[1]WuXi AppTec Co., Shanghai, China*

WP 036 **Development of an LC-MS/MS Method for the Quantitation of Fatty Acid Dicarboxylates, Potential Biomarkers for OATPFunction**; Weiqi Chen[1]; Hong Shen[2]; Yurong Lai[2]; William Humphreys[2]; Jinping Gan[2]; *[1]Bristol-myers Squibb, princeton, NJ; [2]Bristol-Myers Squibb, Princeton, NJ*

WP 037 **Determination of a Double-stranded Small Interfering RNA and its Two Single Strands in Sprague-Dawley Rat Plasma by LC-MS/MS**; Yanfu Ren[1]; Lili Xing[1]; YI TAO[1]; Xinping Fang[1]; Xin Zhang[1]; *[1]WuXi AppTec Co., Shanghai, China*

WP 038 **Differentiating Modes of Drug Induced Liver Injury using Parallel Reaction Monitoring LC-MS**; Michelle R. Robinson[1]; Lei Guo[2]; Raymond J. Gonzalez[1]; Kara M. Pearson[1]; Kevin P. Bateman[1]; Daniel S. Spellman[1]; *[1]Merck Research Laboratories, West Point, PA; [2]Sanofi Genzyme, Cambridge, MA*

WP 039 **Sensitive and Specific Determination of N-Linked Oligomannoses in Mouse Plasma and Brain Tissue Using LC-HRAM Method**; Yuhuan Ji[1]; Qian Li[1]; Jian Shi[1]; John Chen[1]; Chengjie Ji[1]; Laixin Wang[1]; Mo Qatanani[2]; Meng Chen[2]; *[1]NovaBioAssays LLC, Woburn, Massachusetts; [2]Alexion Pharmaceuticals, Lexington, Afghanistan*

WP 040 **Absolute Quantitation of Acetaminophen-Modified HSA by LC-MRM**; Timon Geib[1]; André LeBlanc[1]; Tze Chieh Shiao[1]; Ghazaleh Moghaddam[1]; Amal Guesmi[1]; René Roy[1]; Lekha Sleno[1]; *[1]UQAM, Montreal, QC, Canada, Canada*

WP 041 **SWATH Proteome Phenotyping of Melanoma Identifies Biomarkers of MEK Response and Post Biopsy Survival**; Christoph Krisp[1]; Robert Parker[2]; Dana Pascovici[1]; James Wilmott[3]; John F Thompson[3]; Graham J Mann[3]; Nicholas Hayward[4]; Richard A Scolyer[3]; Mark P Molloy[1]; *[1]Australian Proteome Analysis Facility, Sydney, NSW; [2]Imperial College, London, UK; [3]Melanoma Institute Australia, Sydney, Australia; [4]Oncogenomics Laboratory, QIMR Berghofer Medical Research Institute, Brisbane, Australia*

WP 042 **Phosphoproteins in Extracellular Vesicles as the Candidate Markers for Breast Cancer**; I-Hsuan Chen[1]; Liang Xue[1]; Chuan-Chih Hsu[1]; Juan Sebastian Paez Paez[1]; Li Pan[1]; Hillary Andaluz Aguilar[1]; Michael K Wendt[1]; Anton Iliuk[1]; Jian-Kang Zhu[1]; Andy Tao[1]; *[1]Purdue University, West Lafayette, IN*

WP 043 **Biomonitoring Cooked Meat Carcinogen 2-amino-1-methyl-6-phenylimidazo[4,5-b]pyridine (PhIP) in Human Hair and Prostate by Nano Liquid Chromatography-High Resolution Tandem Mass Spectrometry**; Shun Xiao[1, 2]; Jingshu Guo[1, 2]; Byeong Hwa Yun[1, 2]; Peter W. Villalta[1]; Suprita Krishna[3]; Resha Tejpaul[3]; Paari Murugan[4]; Christopher J. Weight[3]; Robert J. Turesky[1, 2]; *[1]Masonic Cancer Center, University of Minnesota, Minneapolis, MN; [2]Department of Medicinal Chemistry, University of Minnesota, Minneapolis, MN; [3]Department of Urology, University of Minnesota, Minneapolis, MN; [4]Department of Laboratory Medicine and Pathology, University of Minnesota, Minneapolis, MN*

WP 044 **Proteomic Signature of BRCA1-like Triple-Negative Breast Cancers with Homologous Recombination Deficiency**; Youdinghuan Chen[1, 2]; Nicole P. Jenkins[1]; Yue Wang[3]; Johnathan D. Marotti[4]; Chao Cheng[3, 5, 6]; Lucas A. Salas[2]; Brock C. Christensen[2, 3, 6]; Todd W. Miller[3, 6]; Arminja N. Kettenbach[1, 6]; *[1]Department of Biochemistry and Cell Biology, Dartmouth College, Lebanon, NH; [2]Department of Epidemiology, Dartmouth College, Lebanon, NH; [3]Department of Molecular and Systems Biology, Dartmouth College, Lebanon, NH; [4]Department of Pathology and Laboratory Medicine, Dartmouth College, Lebanon, NH; [5]Department of Biomedical Data Science, Dartmouth College, Lebanon, NH; [6]Norris Cotton Cancer Center, Lebanon, NH*

WP 045 **Development of Chemical Isotope Labeling LC-MS for Metabolite Biomarker Discovery of Alzheimer's Disease in a Mouse Model**; Xiaohang Wang[1]; Xinyun Gu[1]; Wei Han[1]; Jing Yang[1]; David Westaway[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB, Canada*

WP 046 **High Sensitivity CZE-ESI-MS Investigations and Applications in Proteomics**; Emily Amenson[1]; Liangliang Sun[2]; Norman J Dovichi[1]; *[1]University of Notre Dame, Notre Dame, IN; [2]Michigan State University, Lansing, MI*

WP 047 **Novel GC-MS Method for the Characterization and Quantification of Short Chain Fatty Acids, Malonaldialdhyde, and Muconic Acid in Biological Samples**; Blake Lynch[1]; Daniel Conklin[1]; Aruni Bhatnagar[1]; Sanjay Srivastava[1]; Pawel Lorkiewicz[2]; *[1]University of Louisville, Louisville, KY; [2]University of Louisville, Louisville, KY*

WP 048 **Targeted Proteomic Characterization of Human Multipotent Stromal Cells Therapeutic Properties**; Miljan Kuljanin[1]; David A. Hess[2, 3]; Gilles A. Lajoie[1]; *[1]Don Rix Protein Identification Facility, Department of Biochemistry, Schulich School of Medicine and Dentistry, University of Western Ontario, London, Ontario; [2]Krembil Centre for Stem Cell Biology, Molecular Medicine Research Group, Robarts Research Institute, London, Ontario; [3]Department of Physiology and Pharmacology, Schulich School of Medicine and Dentistry, University of Western Ontario, London, Ontario*

WP 049 **Intelligent Algorithm using Particle Swarm Optimization (SWARM) with Enhanced Limit of Detection for Large Molecule Applications**; Huy Bui[1]; Christian Klein[2]; Alex Zhu[3]; Alex Mordehai[2]; Gregor Overney[2]; *[1]Agilent Technologies, Santa Clara, CA; [2]Agilent Technologies, Santa Clara, CA; [3]Agilent Technologies, Inc., Wilmington, DE*

WP 050 **High-precision Quantification of Warburg Effect Enzymes in a Comprehensive Panel of Breast Cancer Patient Derived Xenografts**; Robert W. Sprung[1]; Petra Erdmann-Gilmore[1]; Sherri R. Davies[1]; John A. Wrobel[2]; Rose Connors[1]; Yiling Mi[1]; Lisa J. Zimmerman[3]; Daniel C. Liebler[3]; Reid Townsend[1]; *[1]WUSTL, St. Louis, MO; [2]UNC - Chapel Hill, Chapel Hill, NC; [3]Vanderbilt University Medical Center, Nashville, TN*

WP 051 **Clinical Tracers: A Simple, Rapid and Simultaneous LC-MS Method to Measure Stable Isotope Enrichment of Glucose, Glycerol And Palmitic Acid**; Peter J Walter[1]; H. Martin Garraffo[1]; Stephanie Chung[1]; Rebecca J Brown[1]; *[1]NIH, Bethesda, MD*

WP 052 **A Generic Kit-Based Approach for LC-MS/MS Quantification of Urinary Albumin for Clinical Research**; Mary E Lame[1]; Caitlin M Dunning[2]; Paula M Orens[2]; *[1]Waters Technologies Corporation, Milford, MA; [2]Waters Corporation, Milford, MA*

WP 053 **LC-MS/MS Quantification of Urine Glycosaminoglycans in Children with Severe Malaria**; Haoyue Zhang[1]; J. Brice Weinberg[2]; Nicholas M Anstey[3]; Matthew P Rubach[2]; Tsin W Yeo[4]; Salvatore Florence[5]; Esther D Mwaikambo[5]; Donald L Granger[6]; David S Millington[1]; *[1]Duke University Pediatrics , Durham, NC; [2]Duke University and VA Medical Centers, Durham, NC; [3]Menzies School for Health Research and Charles Darwin University, Darwin, Australia; [4]Lee Kong Chian School of Medicine, Nanyang Technological University, Nanyang, Singapore; [5]Hubert Kairuki Memorial University, Dar es Salaam, Tanzania; [6]University of Utah School of Medicine and VA Medical Center, Salt Lake City, UT*

WP 054 **LC-SRM to Quantify Suitable Tau Peptides to Evaluate Animal Model and Follow Disease Progression**; Chloe Bardet[1]; Tanguy Fortin[1]; Rodolphe Billiras[2]; Arnaud François[2]; Valérie Pasteau[2]; Karine Albinet[2]; Gaelle Rollin-jego[2]; Fabrice Iop[2]; Alain Gobert[2]; *[1]Anaquant, Villeurbanne, France; [2]Neuropsychiatry Innovation Therapeutic Pole, Institut de Recherches Servier, Croissy sur Seine, France*

WP 055 **MRM-based Validation Assay for Serum Proteomic Alterations in Meningioma Patients**; Shuvolina Mukherjee[1]; Sujata Wajunj[1]; Purushottam Sutar[2]; Ajit Datar[2]; Aliasgar Moiyadi[3]; Epari Sridhar[3]; Sanjeeva Srivastava[1]; *[1]Indian Institute of Technology Bombay, Mumbai, India; [2]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India; [3]Tata Memorial Hospital, Parel, Mumbai, India*

WP 056 **Quantitation of Orotic Acid in Human Urine on the AB SCIEX API-4000 LC-MS/MS System**; YONG-XI LI[1]; Joshua Froning[1]; Guangchun Zhou[1]; *[1]Medpace Bioanalytical Laboratory, Cincinnati, OH*

WP 057 **Multi-Matrix LC-MS/MS Methods for Quantification of Neurological Biomarkers N-Acetyl Aspartic Acid and Homocarnosine**; Dewakar Sangaraju[1]; Xiao Ding[1]; Sheerin K Shahidi-Latham[1]; *[1]Genentech, Inc, South San Francisco, CA*

WP 058 **A Rapid Measurement of Urinary 6-Sulfatoxymelatonin (aMT6s) as a Biomarker Using HPLC-Tandem Mass Spectrometry**; Tian-Sheng Lu[1]; Guandnong Zhang[1]; Feng Yin[1]; Joshua Froning[1]; Emily Epure[1]; Yong-Xi Li[1]; *[1]Medpace Bioanalytical Laboratory, Cincinnati, OH*

WP 059 **Quantitative HPLC-MS/MS Analysis of Human Apolipoproteins Utilizing SILuMab as a Commercially Available Internal Standard and Standard 96-Well Plates**; Caleb Robinson[1]; Ann Hoffman[1]; Chad D. Christianson[1]; Jennifer S.D. Zimmer[1]; Shane R. Needham[1]; *[1]Alturas Analytics, Inc., Moscow, ID*

WP 060 **An LC-MS/MS Measurement of Cortisol as a Biomarker in Human Urine**; Feng Yin[1]; Andrew Swenson[1]; Emily Epure[1]; Tian-Sheng Lu[1]; Yong-Xi Li[1]; *[1]Medpace Inc., Cincinnati, OH*

WP 061 **Direct Measurement of Serotonin Synthesis as a Predictive Marker of Serotonin Pharmacodynamics and Disease-Induced Dysregulation**; Richard Welford[1]; Magali Vercauteren[1]; Annette Trébaul[1]; Christophe Cattaneo[1]; Doriane Eckert[1]; Marco Garzotti[1]; Patrick Sieber[1]; Jérôme Segrestaa[1]; Rolf Studer[1]; Peter M Groenen[1]; Oliver Nayler[1]; *[1]Actelion Pharmaceuticals, Allschwil*

WP 062 **Analysis of Deuterated Phenanthrene Metabolites in Human Urine by GC-NICI-MS/MS-SRM**; Kai Luo[1]; Viviana Paiano[1]; Steven G. Carmella[1]; Jon B. Hochalter[1]; Naomi Fujioka[1]; Stephen S. Hecht[1]; *[1]University of Minnesota, Minneapolis, MN*

WP 063 **Simultaneous Quantitative Determination of Synthetic Cathinones Enantiomers in Urine and Plasma using GC-NCI-MS**; Rashed Alrumaithi[1]; Mohammad Almeetani[2]; Anas Alaidaros[2]; Adnan Lanjawi[1]; Khaled Alsumaiti[1]; *[1]Dubai Police, Dubai, Dubai; [2]United Arab Emirates University, Al Ain, United Arab Emirates*

WP 064 **Calculating Biological Age Using Label-Free Mass Spectrometry Based Proteomics**; Harris Bell-Temin[1]; Matthew Yousefzadeh[2]; Jessica Snyder[3]; Warren Ladiges[3]; Paul Robbins[2]; Laura Niedernhofer[2]; Nathan A Yates[1]; *[1]University of Pittsburgh School of Medicine, Pittsburgh, PA; [2]The Scripps Research Institute, Jupiter, FL; [3]University of Washington, Seattle, WA*

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WP 065 **Profiling Biochemical Individuality: Human Personal Omics Profiling (hPOP)**; Sara Ahadi[1]; Hannes Roest[1]; Liang Liang[1]; Christie Hunter[2]; Mike Snyder[1]; *[1]Stanford School of Medicine, Stanford, CA; [2]SCIEX, Redwood City, CA*

WP 066 **Characterization of Data-Independent Acquisition (DIA) Capabilities of a Q-TOF Instrument for Complex Proteomics Samples**; Stephanie Kaspar-Schoenefeld[1]; Thomas Kosinski[1]; Romano Hebeler[1]; Pierre-Olivier Schmit[1]; Gary Kruppa[1]; *[1]Bruker Daltonik GmbH, Bremen, Germany*

WP 067 **PepShare Mapper – A Strategy to use Shared Peptides from SWATH-MS to Quantitate Isoforms and Analyze Mixed Species Proteomes**; Christoph Krisp[1]; Jemma Wu[1]; Mark P Molloy[1]; *[1]Australian Proteome Analysis Facility, Sydney, NSW*

WP 068 **Analysis of m/z Distribution of Tryptic Peptides in Various Types Biological Samples, Supporting Generic DIA Strategies**; Faraz Rashid[1]; Manoj Pillai[1]; Dipankar Malakar[1]; *[1]AB SCIEX, Gurgaon, Haryana*

WP 069 **Quantitative Analysis of Proteomic Samples using a Novel Scanning Quadrupole Method**; Sarah Lennon[1]; Gushinder Kaur-Atwal[1]; Erika P Parkinson[2]; Paul J. Skipp[2]; Thérèse McKenna[1]; *[1]Waters Corporation, Wilmslow; [2]Centre for Biological Sciences, University of Southampton, Southampton, UK*

WP 070 **Future Directions for Data-Independent Acquisition Modes Utilising a Scanning Quadrupole on Q-ToF Instruments**; Keith G. Richardson[1]; Jason L. Wildgoose[1]; Chris Hughes[1]; Praveen Harapanahalli[1]; *[1]Waters Corporation, Wilmslow, UK*

WP 071 **Enhancing the Throughput and Robustness of DIA using a 150 µm EASY-Spray Column**; Joshua Nicklay[1]; Kerry M Hassell[1]; Aran Paulus[2]; *[1]Thermo Fisher Scientific, Somerset, NJ; [2]Thermo Fisher Scientific, San Jose, CA*

WP 072 **Utilization of IM-MS Deconvolution for Reduced LC Separation Time Requirements in High-throughput Proteomics**; Michael E. Pettit[1]; Matthew R. Brantley[1]; Fabrizio Donnarumma[2]; Kermit K. Murray[2]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX; [2]Louisiana State University, Baton Rouge, LA*

WP 073 **Building a Community Platform for High-Throughput Data Independent Acquisition Analysis on the Cloud**; Jarrett Egertson[1]; Brian Searle[1, 2]; Sonia Ting[1]; Lindsay K Pino[1]; Han-Yin Yang[1]; Austin Keller[1]; Vagisha Sharma[1]; Brendan MacLean[1]; Michael J MacCoss[1]; *[1]University of Washington, Seattle, WA; [2]Proteome Software, Portland, OR*

WP 074 **A New Approach to Generate High Quality Spectral Libraries and Determine Signal Interference in DIA Experiments**; Antoine Lesur[1]; Petr V. Nazarov[1]; Sang Yoon Kim[1]; Sébastien Gallien[2]; Gunnar Dittmar[1]; Daniel Ayoub[1]; *[1]Proteome and Genome Research Unit, Department of Oncology, Luxembourg Institute of Health, Strassen, Luxembourg; [2]Thermo Fisher Scientific, Courtaboeuf, France*

WP 075 **Data Independent Acquisition with a Fast Scanning, Low Resolution Hybrid Quadrupole-Linear Ion Trap**; Austin Keller[1]; Jarrett Egertson[1]; Brian Searle[1, 2]; Lindsay K Pino[1]; Philip M Remes[3]; Romain Huguet[3]; Michael J MacCoss[1]; *[1]University of Washington, Seattle, WA; [2]Proteome Software, Portland, OR; [3]Thermo Fisher Scientific, San Jose, CA*

WP 076 **Using Orbitrap's Unique Strengths, Combined with DeepDIA's DeepSearch Protocol, to Maximize Sensitivity on DIA-capable Orbitrap Instruments**; Dennis Goldfarb[1]; Gautam Saxena[1]; *[1]DeepDIA, Bethesda, MD*

WP 077 **A Dual Workflow to Improve the Protein Coverage for Plasma Data-Independent Analysis**; Shenyan Zhang[1]; Qin Fu[1]; Vidya Venkatraman[1]; Ronald Holewinski[1]; Jennifer Van Eyk[1]; *[1]Cedars-Sinai Medical Center, Los Angeles, CA*

WP 078 **GPGPU-based Database-Search Engine for Feature Identification with DIA data**; Yu Gao[1]; John R. Yates III[1]; *[1]The Scripps Research Institute, La Jolla, CA*

WP 079 **Structural Elucidation of an Unknown Compound in Avocado Fatty Acid Methyl Esters (FAMEs) Extract Using APGC-HRMS**; Lauren Mullin[1, 2]; Dana Krueger[3]; Melissa Phillips[4]; Sarah Dowd[5]; Joe Romano[1]; Kenneth Rosnack[1]; *[1]Waters Corporation, Milford, MA; [2]Örebro University, Örebro, Sweden; [3]Krueger Food Laboratories Inc, Chelmsford, MA; [4]NIST, Gaithersburg, MD; [5]Waters Corporation, Beverly, MA*

WP 080 **Having a Free Lunch: A Combined DIA+DDA Approach Towards Spectral Library Generation for DIA Analysis using Spectronaut**; Tejas Gandhi[1]; Lynn Verbeke[1]; Oliver M. Bernhardt[1]; Roland Bruderer[1]; Jan Muntel[1]; Lukas Reiter[1]; *[1]Biognosys, Schlieren, Zurich*

WP 081 **Deep Proteomic Profiling using Data Independent Acquisition**; Reta Birhanu Kitata[1, 2, 3]; Pei-Yi Lin[1]; Ching-Tai Chen[4]; Chia-Feng Tsai[5]; Alexey I. Nesvizhskii[6]; Ting-Yi Sung[4]; Yu-Ju Chen[1]; *[1]Institute of Chemistry, Academia Sinica, Taipei City, Taiwan; [2]Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan; [3]Molecular Science and Technology Program, Taiwan International Graduate Program, Academia Sinica, Taipei City, Taiwan; [4]Institute of Information Science, Academia Sinica, Taipei City, Taiwan; [5]Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; [6]Department of Computational Medicine and Bioinformatics and Department of Pathology, University of Michigan Medical School, Ann Arbor, MI*

WP 082 **Data Independent Acquisition of Small Molecules by Resonance Collision Induced Dissociation**; Philip M Remes [1]; Austin Keller[2]; Jarrett Egertson[2]; Richard Johnson[2]; Romain Huguet[1]; Michael J MacCoss[2]; Jae C. Schwartz[1]; *[1]Thermo Fisher Scientific, San Jose, California; [2]University of Washington, Department of Genome Sciences, Seattle, WA*

WP 083 **From Targeted to Untargeted DNA Damage Screening — DNA Adduct "Omics" Analysis by High Resolution Multi-stage Mass Spectrometry**; Jingshu Guo[1, 2]; Peter W. Villalta[1]; Robert J. Turesky[1, 2]; *[1]Masonic Cancer Center, University of Minnesota, Minneapolis, MN; [2]Department of Medicinal Chemistry, University of Minnesota, Minneapolis, MN*

WP 084 **Optimization of SONAR Elevated Energy Ramps Applied to Different Molecule Classes**; Chris Hughes [1]; Lee A Gethings[1]; Jonathan P Williams[1]; Johannes P.C. Vissers[1]; James I Langridge[1]; *[1]Waters, Manchester , UK*

WP 085 **Comprehensive DIA on a Q-ToF Instrument for Discovery and Quantitative Analysis Utilising a Scanning Quadrupole**; Jason Wildgoose[1]; Keith Richardson[1]; Martin R. Green[1]; *[1]Waters Corporation, Wilmslow, UK*

WP 086 **De novo DIA Analysis (DDA)**; Richard S. Johnson[1]; Brian Searle[2]; Austin Keller[2]; Michael J MacCoss[2]; *[1], Mercer Island, WA; [2]University of Washington Genome Sciences, Seattle, WA*

WP 087 **Universal Data-Independent LC-MS/MS Workflow for Host Cell Protein Characterization and Quantification in Biopharmaceutical Product Purification Process**; Lei Xiong[1]; Yihan Li[1]; Stephen Tate[2]; Todd Stawicki[3]; Edita Botonjic-Sehic[4]; Mark Schofield[4]; Vincent Ravault[5]; Sean McCarthy[3]; Hua-Fen Liu[1]; *[1]SCIEX, Redwood City, CA; [2]SCIEX, Concord, ON, Canada; [3]SCIEX, Framingham, MA; [4]Pall Corporation, Westborough, MA; [5]Pall Corporation, Cergy, France*

WP 088 **Two-Dimensional Mass Spectrometry in a Linear Ion Trap**; Maria A. van Agthoven[1]; Christopher A. Wootton[1]; Peter B. O'Connor[1]; *[1]University of Warwick, Coventry, Midlands, UK*

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WP 089 **Bitransformation and Metabolic Profile of the Roots of the Polygala with Intestinal Microflora In Vitro by UPLC-MS Method**; Zhiqiang Liu[1]; Guifang Feng[2]; Shu Liu[1]; *[1]National Center for Mass Spectrometry in Changchun & Key Laboratory for Traditional Chinese Medicine Chemistry and Mass Spectrometry of Jilin province & Chemical Biology Laboratory, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun, China; [2]University of Science and Technology of China, Hefei, China*

WP 090 **In vitro Investigation of Metabolic Profiling of Newly Developed Topoisomerase Inhibitors (Ethyl Fluorescein Hydrazones, EtFLHs) in RLMs by LC-MS/MS**; Adnan A Kadi[1]; Nasser S Al-Shakliah[1]; A. F. M. Motiur Rahman[1]; *[1]King Saud University, Riyadh, Riyadh*

WP 091 **A Rapid and Sensitive LC-HRMS Method for Detection of Glutathione-Trapped Reactive Metabolites using a High-Resolution Orbitrap System**; Zhican Wang[1]; Ying Fang[1]; Dan Rock[1]; Ji Ma[1]; *[1]Amgen, South San Francisco, CA*

WP 092 **Simultaneous Determination of Metabolic Stability and Metabolite Identification using a High-Resolution Mass Spectrometry**; Zhican Wang[1]; Min Jiang[1]; Chi-Chi Peng[1]; Dan Rock[1]; Ji Ma[1]; *[1]Amgen, South San Francisco, CA*

WP 093 **Strain and Sex Differences in Metabolism in Rats: Assessment of Buspirone Metabolism by High Resolutionlcms/MS Analysis**; Rutali R. Brahme[1]; Jennifer L. Dumouchel[1]; Upendra A. Argikar[1]; *[1]Novartis Institutes for BioMedical Research, Cambridge, MA*

WP 094 **Profiling of In Vitro and In Vivo Metabolites of Novel TKIs using LC-MS/MS Method: Metabolic Stability and Bioactivation Pathway Elucidation**; Adnan A. Kadi[1]; Hany W. Darwish[1, 2]; Mohamed W Attwa[1, 2]; Sawsan M. Amer[2]; *[1]College of Pharmacy, King Saud University, Riyadh, Saudi Arabia; [2]Faculty of Pharmacy, Cairo University, Cairo, Egypt*

WP 095 **A New Method for Analyzing MSe/All Ions Fragmentation in Xenobiotic Metabolism Studies**; Richard Lee[1]; Vitaly Lashin[2]; Alexandre Sakarov[2]; Andrey Paramonov[2]; *[1]ACD/Labs, Burlington, ON, Canada; [2]ACD/Labs, Moscow, Russia*

WP 096 **A New Biotransformation Prediction Engine Integrated into a Metabolite Identification Solution**; Richard Lee[1]; Rytis Kubilius[2]; Vitaly Lashin[3]; Alexandre Sakarov[3]; Andrey Paramonov[3]; *[1]ACD/Labs, Burlington, ON, Canada; [2]ACD/Labs, Vilnius, Lithuania; [3]ACD/Labs, Moscow, Russia*

WP 097 **Revisit Metabolism and Bioactivation of Ketoconazole using LC-MS-Based Metabolomics**; Ju-Hyun Kim[1]; Won-Gu Choi[1]; Hye Suk Lee[1]; *[1]College of Pharmacy, The Catholic University of Korea, Bucheon-si, South Korea*

WP 098 **Use of HILIC Chromatography for the Identification of Metabolites of Polar Drugs by HPLC-MS/MS**; Joshua L. Johnson[1]; Adam Amaral[1]; Jiansheng Haung[1]; Ying Liu[1]; Mohammad Shadid[1]; Amin Kamel[1]; *[1]Biogen, Cambridge, MA*

WP 099 **Novel Software Algorithm iMassFrag to Automate Drug Metabolite Identification and Mass Spectral Interpretation**; Siwei Li[1]; Jing Lu[1]; Duxin Sun[1]; *[1]University of Michigan, Ann Arbor, MI*

WP 100 **Fast and Comprehensive Detection and Characterization of Cyclic Peptide Metabolites using Software-Aided Data Processing Tools**; Ming Yao[1]; Eva Duchoslav[2]; Li Ma[1]; Silvi Chacko[1]; Mingshe Zhu[1]; *[1]Bristol-Myers Squibb, Princeton, New Jersey; [2]SCIEX, Concord, ON, Canada*

WP 101 **Dipyridamole High Throughput Analysis of Drug Metabolism Cells Assay using LDTD-MS/MS**; Jean Lacoursiere[1]; Serge Auger[1]; Pierre Picard[1]; *[1]Phytronix Technologies, Québec, QC, Canada, Canada*

WP 102 **Application of iMassFrag, a Novel Mass Spectral Interpretation Algorithm, to Structural Elucidation of Oxidative Drug Metabolites**; Silvi Chacko[1]; Siwei Li[2]; Xiaoliang Zhuo[1]; Weiping Zhao[1]; Duxin Sun[2]; Mingshe Zhu[1]; *[1]Bristol-Myers Squibb, Princeton, New Jersey; [2]University of Michigan, Ann Arbor, MI*

WP 103 **Development of a Sensitive and Selective High Resolution Accurate Mass LC-SIM for the Detection of Oligonucleotides in Biological Matrices**; Heng-Keang Lim[1]; Jie Chen[1]; Salter Rhys[1]; *[1]Janssen Pharmaceuticals R&D, Spring House, PA*

WP 104 **A Metabolite ID Workflow on a Small Footprint Benchtop Q-TOF Mass Spectrometer with Automated Software Structure Generation**; Shaokun Pang[1]; Ian Moore[2]; *[1]SCIEX, Redwood City, CA; [2]SCIEX, Concord, ON, Canada*

WP 105 **Label Free High Throughput Screening of Amino Acid Based Assays: Old Tricks, New Speed using LDTD-MS/MS**; Pierre Picard[1]; Sylvain Letarte[1]; Serge Auger[1]; Jean Lacoursiere[1]; *[1]Phytronix Technologies, Inc., Quebec, QC, Canada*

WP 106 **High-Throughput and Automated Software Workflow Strategies for Small Molecule Identification and Characterization Using a High Resolution Q-TOF Mass Spectrometer**; Alina Dindyal-Popescu[1]; Iris Shek[1]; Mohammed Jooyandeh[1]; Ian Moore[1]; Eva Duchoslav[1]; *[1]SCIEX, Concord, ON, Canada*

WP 107 **The Application of Research Grade MetabolitePilot™ Software for the Determination of Exenatide Catabolites using HRAM with SWATH Acquisition**; Jeff Plomley[1];

Yi Zhang[2]; Eva Duchoslav[3]; DANIEL Villeneuve[1]; Kevork Mekhssian[1]; Anahita Keyhani[1]; *[1]Algorithme Pharma an Altasciences company, Laval, QC, Canada; [2]Sciex, Framingham, MA; [3]Sciex, Concord, ON, Canada*

WP 108 **Horses For Courses – A Comparison of SONAR and Other Data-Independent Acquisition Strategies for Drug Metabolism and Pharmacokinetics**; Russell Mortishire-Smith[1]; Jayne Kirk[1]; Mark Wrona[2]; Sherri Naughton[2]; Kirsten Craven[1]; *[1]Waters Corporation, Wilmslow, UK; [2]Waters Corp, Milford, MA*

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WP 109 **Toxic Metal Accumulation and Speciation of Foodstuffs in Aquaponics Systems using HPLC and ICP-MS**; Skyler Smith[1]; Megan Schmale[1]; Julio A. Landero Figuero[1]; *[1]University of Cincinnati, Cincinnati,OH*

WP 110 **Quantitative Determination of Heavy Metals in Ayurvedic Tablets using ICPMS**; Ankush Bhone[1]; Sampada Khopkar[1]; Mangesh Pawar[1]; Amol Shinde[1]; Ajit Datar[1]; Jitendra Kelkar[1]; Pratap Rasam[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

WP 111 **Quantitative Determination of Heavy Metals in Whole Blood using Inductively-Coupled-Plasma-Mass Spectrometry (ICPMS) by Microwave Digestion and Dilution Technique**; Sampada Khopkar[1]; Mangesh Pawar[1]; Amol Shinde[1]; Ankush Bhone[1]; Ajit Datar[1]; Jitendra Kelkar[1]; Pratap Rasam[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

WP 112 **Exposure and Safety Studies of Herbal Supplements from the United States and Nigeria by Inductively Coupled Plasma Mass Spectrometry (ICPMS)**; Olujide Akinbo[1]; Kyle Colston[1]; *[1]Butler University, Indianapolis, IN*

WP 113 **Evaluating Heavy-Metal Induced Stress in Aquaponics Systems through Phytochelatins**; Megan Schmale[1]; Julio A. Landero Figuero[2]; *[1]University of Cincinnati, Cincinnati , OH; [2]University of Cincinnati, Cincinnati, OH*

WP 114 **Elemental Profiling to Combat Illegal Wildlife Trade**; Simin D. Maleknia[1]; Keith Leggett[2]; Chris Marjo[2]; Mike Letnic[2]; *[1]University of New South Wales, Sydney , NSW; [2]University of New South Wales, Sydney, Australia*

WP 115 **Inductively Coupled Plasma-Mass Spectrometry Coupled with Solid Phase Microextraction for Simultaneous Determination of Heavy Metals in Natural Water**; Ahmad Rohanifar[1]; Lidia B. Rodriguez[1]; Amila M. Devasurendra[1]; Niloofar Alipourasiabi[1]; Jon R. Kirchhoff[1]; *[1]University of Toledo, Toledo, OH*

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WP 116 **Phosphoproteomic Approach for Deciphering Signaling Pathways in Chalmdyomonas Reinhardtii**; Emily G. Werth[1]; Evan W. McConnell[1]; Inmaculada Concepcion Couso Lianez[2]; James G. Umen[2]; Leslie M Hicks[1]; *[1]UNC Chapel Hill, Chapel Hill, NC; [2]Donald Danforth Plant Science Center, St. Louis, MO*

WP 117 **Thin-Film vs Powder Lignin Pyrolysis Analyzed byμPy-GC-dAPCI-TOFMS with In-Source CID**; Evan Larson[1]; Carolyn Hutchinson[1]; Young-Jin Lee[1]; *[1]Iowa State University, Ames, IA*

WP 118 **Lipid Characterization in Genetically Engineered Yarrowia lipolytica by Desorption Electrospray Ionization Mass Spectrometry**; John Lin[1]; Lauren T. Cordova[2]; Hal S. Alper[2]; Livia S. Eberlin[1]; *[1]Department of Chemistry, The University of Texas at Austin, Austin, TX; [2]McKetta Department of Chemical Engineering, The University of Texas at Austin, Austin, TX*

WP 119 **Real-Time Monitoring of Single Particle Herbaceous and Woody Biomass in μPy-dAPCI-TOF MS**; Carolyn Hutchinson[1]; Evan Larson[1]; Young Jin Lee[1]; *[1]Iowa State University, Ames, IA*

WP 120 **The Investigation of the Bio-Oil Produced by Hydrothermal Liquefaction of Different Microalgae Strains using Fourier Transform Mass-Spectrometry and Hydrogen/Deuterium Exchange**; Gleb Vladimirov[1, 2]; Yury Kostyukevich[1, 2, 3, 4]; Igor Popov[2, 3]; Mikhail Vlaskin[5]; Nadezhda Chernova[6]; Sophia Kiseleva[6]; Eugene Nikolaev[1, 2, 3]; *[1]Skolkovo Institute of Science and Technology, Skolkovo, Russia; [2]Institute of Energy Problems of Chemical Physics Russian Academy of Sciences, Moscow, Russia; [3]Moscow Institute of Physics and Technology (State University), Dolgoprudnyj, Russia; [4]Institute of Biochemical Physics Russian Academy Of Sciences, Moscow, Russia; [5]Joint Institute for High Temperatures of the Russian Academy of Sciences, Moscow, Russia; [6]M.V. Lomonosov Moscow State University, Moscow, Russia*

WP 121 **Characterizing the Range and Specificity of Substrate-Specific Extracellular Enzymes in Caldicellulosiruptor Bescii**; Suresh Poudel[1, 2]; Richard J Giannone[2]; Mirko Basen[3]; Farris Poole[3]; Robert Kelly[4]; Michael W Adams[3]; Robert L Hettich[5]; *[1]University of Tennessee, Knoxville, TN; [2]Oak Ridge National Lab, Oak Ridge, TN; [3]University of Georgia, Athens, GA; [4]North Carolina State University, Raleigh, NC; [5]Oak Ridge National Laboratory, Oak Ridge , TN*

WP 122 **Experimental Study of the Combustion Kinetics of the Monoterpenes α-Pinene, β-Pinene, and Myrcene in Flames by Photoionization Time-of-Flight Mass Spectrometry**; Thomas Bierkandt[1]; Tina Kasper[1]; *[1]University of Duisburg-Essen, Duisburg, Germany*

WP 123 **Study of Douglas and Miscanthus Wood Material and Miscanthus Biochar by LDI FT-ICR MS**; Frédéric Aubriet[1]; Thierry Ghislain[2]; Vincent Carré[1]; Yann Le Brech[2]; Ghislain Mauviel[2]; Anthony Dufour[2]; *[1]Université de Lorraine - LCP-A2MC, Metz, France; [2]Université de Lorraine, LRGP, Nancy, France*

WP 124 **A Multi-Omic Approach to Decipher the Regulatory Mechanisms Controlling Lipid Production in Oleaginous Yeast for the Enhanced Production of Biofuels**; Richard J. Giannone[1]; Nancy L. Engle[1]; Robert L. Hettich[1]; Daniel A. Jacobson[1]; Timothy J. Tschaplinski[1]; Daniel M. Close[1]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN*

WP 125 **Diagnostic Tools for Measuring Early Chemical Signatures of Algae Pond Crash** ; Curtis Mowry[1]; Matthew W. Moorman[1]; Adam S. Pimentel[1]; Jerilyn A. Timlin[1]; Todd W. Lane[2]; Carolyn L. Fisher[2]; Stephen M. Anthony[1]; Komandoor Achyuthan[2]; *[1]Sandia National Laboratories, Albuquerque, NM; [2]Sandia National Laboratories, Livermore, CA*

WP 126 **Comparison of Product Distributions from Fast Pyrolysis of Genetic Variants of Poplar by Using a Pyroprobe Inside an APCI Source**; Lan Xu; *Purdue University, West Lafayette, IN*

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WP 127 **Targeted and Non-Targeted Metabolomics to Study Developmental Neurotoxicity of Biocides - Metabolomic Pathway Analysis Reveals Developmental Neurotoxic Effects of Pesticides**; Pim Leonards[1]; Aiko Barsch[2]; Magdalene Reinkensmeier[2]; Andrew Baca[3]; Heiko Neuweger[2]; *[1]Environment & Health, VU University of Amsterdam, Amsterdam, Netherlands; [2]Bruker Daltonics, Bremen, Germany; [3]Bruker Daltonics, Fremont, CA*

WP 128 **Monitoring of human urinary metabolites of biogenic volatile organic compounds using UPLC-MS/MS**; Zhengzhi Xie[1]; Pawel Lorkiewicz[1]; Ray Yeager II[1]; Rachel Keith[1]; Sanjay Srivastava[1]; Aruni Bhatnagar[1]; *[1]University of Louisville, Louisville, KY*

WP 129 **Meet Stringent Detection Requirements for All 13 4-Nonylphenol Isomers in Water using GCMS-SIM**

and a High Efficiency Ion Source; Katsura Sekiguchi[1]; Kamila Kalachova[2]; Melissa Churley [3]; Harry Prest[4]; *[1]Agilent Technologies Japan, Ltd., Hachioji Site, Japan; [2]Agilent Technologies Sales & Services GmbH & Co. KG, Waldbronn, Germany; [3]Agilent Technologies, Inc., Santa Clara, CA; [4]Agilent Technologies Inc., Santa Clara, CA*

WP 130 **Quantification of Persistent Organic Pollutants in Human Blood Using Stir Bar Sorptive Extraction-GC triple Quad-Isotope Dilution Mass Spectrometry**; Weier Hao[1]; Anthony Macherone[2]; H. M. Skip Kingston[1]; Edward Pfannkoch[3]; Matt Pamuku[4]; Stephen Benchouk[5]; *[1]Duquesne University, Pittsburgh, PA; [2]Agilent Technologies, Inc., Santa Clara, CA; [3]GERSTEL, Inc., Linthicum, MD; [4]Applied Isotope Technologies Company, Pittsburgh, PA; [5]Infinity Life Center, Honolulu, HI*

WP 131 **Analytical Method Development for Widely Targeted Perfluoroalkyl Acids (PFAAs) and their Precursors in Plasma using Multi-Gradient Eluent System by LC-MS/MS**; Jun Watanabe[1]; Toshikazu Minohata[1]; Tairo Ogura[2]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Shimadzu Scientific Instr., Columbia, MD*

WP 132 **An APGC-MS MRM Method for the Quantitation of Common Acrylates in a Single Method**; Vincent Pagnotti[1]; Benjamin Cooley[1]; Conner Stultz[2]; Frank Dorman[2]; *[1]PPG Industries, Allison Park, PA; [2]Pennsylvania State University, State College, PA*

WP 133 **Materials and Methods for Measuring the Non-Protein Amino Acid BMAA in Proteins**; David C Muddiman[1]; Philip L Loziuk[1]; Lauren C Nufer[1]; Yasamin Moazami[1]; Joshua G Pierce[1]; Denis Fourches[1]; Scott J Mellors[2]; J. Michael Ramsey[3]; *[1]North Carolina State University, Raleigh, NC; [2]908 Devices, Inc., Carrboro, NC; [3]UNC, Chapel Hill, NC*

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WP 135 **Determination of Trace Levels of Microcystins in Aqueous Samples by Direct Injection LC-MS/MS**; Paul C. Winkler[1]; Craig Butt[2]; April Quinn-Paquet[2]; *[1]SCIEX, Framingham, MA; [2]SCIEX, Framingham, MA*

WP 136 **Molecular Characterization of Water-Soluble Organic Carbon (WSOC) from Biomass Burning Aerosol using Ultrahigh Resolution Orbitrap Elite Mass Spectrometry**; Elena N Kirillova[1]; Vera Samburova[2]; Chiranjivi Bhattarai[2]; Deep Sengupta[2]; Hans Moosmüller[2]; Andrey Khlystov[2]; Lynn R Mazzoleni[1]; *[1]Michigan Technological University, Houghton, MI; [2]Desert Research Institute, Reno, NV*

WP 137 **Molecular Characterization of Ambient and Laboratory Biomass Burning Influenced Aqueous Phase Secondary Organic Aerosol Utilizing Ultrahigh Resolution Mass Spectrometry**; Matthew Brege[1]; Marco Paglione[2]; Stefania Gilardoni[2]; Stefano Decesari[2]; Maria Cristina Facchini[2]; Lynn R Mazzoleni[1]; *[1]Michigan Technological University, Houghton, MI; [2]Italian National Research Council, Bologna, Italy*

WP 138 **Determination of Estrogens in Water by Temperature-Controlled Liquid Phase Microextraction Combined with Gas Chromatography-Tandem Mass Spectrometry**; Yi-Yu Chen[1]; Chung-Yu Chen[1]; Maw-Rong Lee[1]; *[1]National Chung-Hsing University, Taichung*

WP 139 **A Rapid, Robust Microcystin Online Concentrion LC/MS/MS Method**; Judy Westrick[1]; Johnna Birbeck[1]; *[1]Wayne State University, Detroit, MI*

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WP 227 **High-Detail Analysis of Plasma Glycoprotein Microheterogeneity by Hybrid Mass Spectrometry Approaches**; Vojtech Franc[1]; Yang Yang[1]; Albert J. R. Heck[1]; *[1]Utrecht University, Utrecht, NE*

WP 228 **Effect of Sialic Acids on N-glycan Release Kinetics by PNGase F**; Naglaa Sheiba[1]; Ron Orlando[1]; *[1]CCRC, University of Georgia, Athens, GA*

WP 229 **Quantitative Glycoproteomics in Complex Samples using Soft Fragmentation**; Miloslav Sanda[1]; Petr Kozlik[1, 2]; Nathan J Edwards[3]; Radoslav Goldman[1, 3]; *[1]Georgetown University, Lombardi Cancer Center, Washington, DC; [2]Charles University, Faculty of Science, Department of Analytical Chemistry, Prague, Czech Republic; [3]Georgetown University, Department of Biochemistry and Molecular & Cellular Biology, Washington, DC*

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WP 231 **In-Depth Site-Specific Glycan Microheterogeneity Characterization with Reversed-Phase Chromatographic Prefractionation Followed by Capillary Zone Electrophoresis-Electrospray Ionization Tandem Mass Spectrometry Analysis**; Yanyan Qu[1]; Liangliang Sun[2]; Zhenbin Zhang[1]; Norman J Dovichi[1]; *[1]Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN; [2]Department of Chemistry, Michigan State University, East Lansing, MI*

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WP 233 **pGlyco 2.0 Enables Precision Glycoproteomics by using Comprehensive Quality Control and One-Step Mass Spectrometry for Intact Glycopeptide Identification**; Mingqi Liu[1]; Wen-Feng Zeng[2]; Wei-qian Cao[1]; Chao Liu[2]; Si-Min He[2]; Peng-Yuan Yang[1]; *[1]Fudan University, Shanghai, China; [2]Key Lab of Intelligent Information Processing of Chinese Academy of Sciences (CAS), Beijing, China*

WP 234 **Enhancing Glycopeptide MS Performance through Derivatization with a Novel Rapid Derivatization Reagent**; William Alley[1]; Brad Williams[2]; Ying Qing Yu[1]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Beverly, MA*

WP 235 **Deep Sequencing of Proteoglycans**; Le Meng[1]; Joshua A. Klein[2]; Joseph Zaia[1]; *[1]Boston University School of Medicine, Boston, MA; [2]Boston University, Boston, MA*

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WP 237 **Evaluation of Electron Transfer Dissociation Reagents for Analysis of N-Glycosylated Peptides**; Maia I. Kelly[1]; Eric D. Dodds[1]; *[1]University of Nebraska - Lincoln, Lincoln, NE*

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WP 245 **Applying a Novel Informatics Approach to Study Site-Specific Urinary Protein N-Glycosylation in the Context of Urinary Tract Infection (UTI)**; John Froehlich[1, 2]; Peter Warren[1]; Shannon DiMartino[1]; Richard S Lee[1, 2]; *[1]Boston Children's Hospital, Boston, MA; [2]Harvard Medical School, Boston, MA*

WP 246 **Quantitation of Human Antibodies with Synthetic Glycopeptides**; Rini Roy[1]; Emy Komatsu[1]; Helene Perreault[1]; *[1]University of Manitoba, Winnipeg, MB*

WP 247 **Profiling of Site-specific N-Glycosylation in Human Serum by Analyses of N-linked Glycans And Glycosite-containing Peptides (NGAG)** ; Shisheng Sun[1, 2]; Yingwei Hu[1]; Shadi Toghi Eshghi[1]; Yang Liu[1]; PUNIT SHAH[1]; Jing Chen[1]; Hui Zhang[1]; *[1]Johns Hopkins University, Baltimore, MD; [2]Northwest University, Xi'an, China*

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WP 249 **Separation and Characterization of Fab and Fc Fragments from Swine Immunoglobulin G (IgG) Papain Digests by MALDI-MS**; Claudia Nelson[1]; Emy Komatsu[1]; Helene Perreault[1]; *[1]University of Manitoba, Winnipeg, MB*

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WP 254 **Carbohydrate Sequencing Complete with Spectral Documentation by MSn**; Vernon Reinhold[1]; Qing Guo[2]; David Ashline[2]; *[1]University of New Hampshire, Durham, NH; [2]University of New Hampshire, Durham, NH*

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WP 257 **Evolution and Evaluation of a Modular Automation Platform for HDX MS**; Alfonso Espada[1]; Ruben Haro[1]; Cristina Sayago[1]; Jesus Castanon[1]; Bruce D pascal[2]; Patrick R Griffin[2]; Jeffrey A. Dodge[3]; Michael J Chalmers[4]; *[1]Lilly S.A., Alcobendas, Madrid; [2]The Scripps Research Institute, Jupiter, FL; [3]Eli Lilly and Company, Indianapolis, IN; [4]Eli Lilly and Company, Indianapolis, IN*

WP 258 **Antibody Aggregate Interface Mapping by Hydrogen Deuterium Exchange Mass Spectrometry using a Customized Automation Instrument**; Qian Zhang[1]; Hui Xiao[1]; Shailin Patel[1]; Chen Li[1]; Ning Li[1]; *[1]Regeneron Pharmaceuticals, Tarrytown, NY*

WP 259 **Optimizing Electron Transfer Dissociation Conditions for Hydrogen/Deuterium Exchange Mass Spectrometry and Its Application to the Study of Protein Conformation**; Terry Zhang[1]; Stephane Houel[2]; Jonathan Josephs[1]; *[1]ThermoFisher, San Jose, CA; [2]Thermo Fisher Scientific, San Jose, CA*

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WP 263 **Sparse Representation for Hydrogen Exchange Mass Spectrometry (HX-MS) Data by using LASSO Optimization**; Yuqi Shi[1]; Jarod V. Hart[2, 3]; David D. WEIS[1, 4]; *[1]Department of Chemistry, University of Kansas, Lawrence, KS; [2]Higuchi Biosciences center, University of Kansas, Lawrence, KS; [3]Department of Mathematics, University of Kansas, Lawrence, KS; [4]Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS*

WP 264 **Characterizing the Forward- and Backward- Hydrogen/Deuterium Exchange of Hydroxyls Resulting from Residual Solvent Vapors in Electrospray Sources**; H. Jamie Kim[1]; Marina R. Mulenos[1]; Tara Liyanage[1]; Elyssia S Gallagher[1]; *[1]Baylor University, Waco, TX*

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WP 267 **Automated Hydrogen-Deuterium Exchange Analysis of Intact Proteins by Top-Down Fragmentation using Electron Transfer Dissociation**; Malcolm Anderson[1]; Laetitia Florence Denbigh[1]; Keith Fadgen[2]; Michael Eggertson[2]; *[1]Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK; [2]Waters Corp, Milford, MA*

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WP 269 **Probing Membrane Protein Conformational Dynamics using HDX-MS**; Yingrong Xu[1]; Jill Chrencik[1]; Kimberly F. Fennell[1]; Laura Byrnes[1]; Justin Hall[1]; Xiayang Qiu[1]; Graham West[1]; *[1]Pfizer Inc., Groton, CT*

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WP 272 **Low Temperature Hydrogen Exchange Microchip Capillary Electrophoresis-Mass Spectrometry**; Kristina M. Herrera[1]; J. Michael Ramsey[1]; *[1]UNC - Chapel Hill, Chapel Hill, NC*

WP 273 **Supercharging for Improved ECD/ETD-Based Hydrogen/Deuterium Exchange Mass Spectrometry**; Qingyi Wang[1]; Kristina I Håkansson[1]; *[1]University of Michigan Chemistry Department, Ann Arbor, MI*

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of Biochemistry, Vanderbilt University, Nashville, TN; [4]Department of Chemistry, Vanderbilt University, Nashville, TN; [5]Institute of Chemical Technologies and Analytics (CTA), TU Wien, Vienna, Austria; [6]Department of Pathology, Microbiology and Immunology, Vanderbilt University School of Medicine, Nashville, TN; [7]United States (U.S.) Department of Veterans Affairs, Tennessee Valley Healthcare System, Nashville, TN; [8]Department of Pharmacology, Vanderbilt University, Nashville, TN; [9]Department of Medicine, Vanderbilt University, Nashville, TN

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WP 279 **Distilling Knowledge from Data: MS Data Analysis using ChemDistiller**; Ivan Laponogov[1]; Noureddin M H Sadawi[1]; Dennis A Veselkov[1]; Dieter Galea[1]; Kirill A Veselkov[1]; *[1]Imperial College London, London, UK*

WP 280 **Advanced Computer Vision Based Registration of Imaging Mass Spectrometry Data in Multi-Modal Experiments**; Nico Verbeeck[1]; Jeffrey Spraggins[2, 3, 4]; Nathan Heath Patterson[2, 3]; Junhai Yang[2, 3]; Etienne Waelkens[5, 6]; Richard M. Caprioli[2, 3, 4, 7, 8]; Raf Van de Plas[1, 2, 3]; *[1]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [2]Mass Spectrometry Research Center (MSRC), Vanderbilt University, Nashville, TN; [3]Department of Biochemistry, Vanderbilt University, Nashville, TN; [4]Department of Chemistry, Vanderbilt University, Nashville, TN; [5]Dept. of Cellular and Molecular Medicine, KU Leuven, Leuven, Belgium; [6]Sybioma, KU Leuven, Leuven, Belgium; [7]Department of Pharmacology, Vanderbilt University, Nashville, TN; [8]Department of Medicine, Vanderbilt University, Nashville, TN*

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WP 282 **Improved Spatial Resolution IR-MALDESI Mass Spectrometry Imaging**; Mark Bokhart[1]; Jeffrey Manni[2]; Måns Ekelöf[1]; Milad Nazari[1]; David C. Muddiman[1]; *[1]North Carolina State University, Raleigh, NC; [2]JGM Associates Inc., Burlington, MA*

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WP 284 **A Pneumatically Assisted Nanospray Desorption Ionization (nano-DESI) Source for Enhanced Metabolite Imaging from Tissue**; Kyle D Duncan[1]; Hilde-Marléne Bergman[1]; Ingela Lanekoff[1]; *[1]Uppsala University, Uppsala , Sweden*

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WP 287 **Development of an Imaging FT-ICR-MS with SIMS, FIB-SEM, and Post-Ionization Capabilities for Biological Applications**; Matthew Brantley[1]; Ian G. M. Anthony[1]; Raul A. Villacob[1]; Carter Lantz[1]; Adam R. Floyd[1]; Christina A. Gaw[1]; Scott Koziol[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

WP 288 **Development of an Optical System for Uniform Laser Irradiation in Stigmatic Imaging Mass Spectrometry**; Yuma Tsurumoto[1]; Hisanao Hazama[1]; Kunio Awazu[1, 2, 3]; *[1]Graduate School of Engineering, Osaka University, Suita, Japan; [2]Graduate School of Frontier Biosciences, Osaka University, Suita, Japan; [3]Global Center for Medical Engineering and Informatics, Osaka University, Suita, Japan*

WP 289 **A Monte-Carlo Approach To Automated Ion Trajectory Calculations for Optimization of an Imaging FT-ICR MS with Post-Ionization Capabilities**; Raul Villacob[1]; Matthew R. Brantley[1]; Ian G.M. Anthony[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

WP 290 **Simultaneous Imaging of Small Metabolites, Lipids and Proteins from Biological Tissues under Ambient Conditions Using Laser Electrospray Mass Spectrometry**; Fengjian Shi[1]; Rachel J. Parise[1]; Evan M. Lutton[2]; Servio H. Ramirez[2]; Robert J. Levis[1]; *[1]Department of Chemistry, Temple University, Philadelphia, PA; [2]Lewis Katz School of Medicine, Temple University, Philadelphia, PA*

WP 291 **Multimodal Chemical and Functional Imaging of Nanoscale Transformations in Ferroelectric Thin Films**; Anton Ievlev[1]; Chance C. Brown[2]; Petro Maksymovych[2]; Sergei V. Kalinin[2]; Olga S. Ovchinnikova[2]; *[1]Oak Ridge National Lab, Oak Ridge, TN; [2]Oak Ridge National Laboratory, Oak Ridge , TN*

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Maastricht University, Maastricht, Netherlands; [3]Department of Pathology, Maastricht University, Maastricht, Netherlands

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WP 295 **Phosphopeptide enhancement in MALDI IMS Experiments**; Hyojik Yang[1, 2]; Jeremy L. Norris[1, 2, 3]; Kevin L. Schey[1, 2]; Jeffrey Spraggins[1, 2, 3]; Richard M. Caprioli[1, 2, 3, 4]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Biochemistry, Vanderbilt University, Nashville, TN; [3]Department of Chemistry, Vanderbilt University, Nashville, TN; [4]Department of Pharmacology and Medicine, Vanderbilt University, Nashville, TN*

WP 296 **Modified TiO2 Monolith for Selective Imprint Imaging of Brain Tissue by Laser Desorption/Ionization-Mass Spectrometry**; Qian Wu[1]; Stanislav S. Rubakhin[1]; Jonathan V. Sweedler[1]; *[1]Department of Chemistry and the Beckman Institute, University of Illinois at Urbana−Champaign, Urbana, IL*

WP 297 **Understanding the Laser Desorption Ionization Mechanisms of Lipids from Tissue Sections After Matrix Deposition by Sublimation**; Nicolas Elie[1]; Sebastiaan Van Nuffel[1]; Alain Brunelle[1]; Pierre Chaurand[1, 2, 3]; *[1]CNRS, Institut de Chimie des Substances Naturelles, Gif sur Yvette, France; [2]University of Montreal, Montreal, QC, Canada; [3]Université Paris-Saclay, Saint-Aubin, France*

WP 298 **Insect Neuropeptide MALDI Imaging: Simultaneous Analysis and Localization with Spatial Resolution at Micrometer Scale**; Alice Ly[1]; Lapo Ragionieri[2]; Sander Liessem[2]; Michael Becker[3, 4]; Soeren-Oliver Deininger[3]; Reinhard Predel[2]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]University of Cologne, Cologne, Germany; [3]Bruker Daltonics, Bremen, Germany; [4]Boehringer Ingelheim GmbH, Biberach, Germany*

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WP 302 **Sample Preparation of the Corn Seed Tissues to Prevent Analyte Relocations for MS imaging**; Sohee Yoon[1]; Shin-Hye Kim[1]; Tae Geol Lee[1]; Jeongkwon Kim[2]; *[1]Korea Research Institute of Standards and Science, Daejeon; [2]Chung Nam National University, Daejeon, South Korea*

WP 303 **Global Lipidomic Changes Associated with MALDI Matrices using MALDI FTICR Imaging Mass Spectrometry**; William J. Perry[1, 2]; Jeffrey M. Spraggins[1, 2, 3]; Raf Van de Plas[1, 3, 4]; Richard M. Caprioli[1, 2, 3, 5, 6]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Chemistry, Vanderbilt University, Nashville, TN; [3]Department of Biochemistry, Vanderbilt University, Nasvhille, TN; [4]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [5]Department of Pharmacology, Vanderbilt University, Nashville, TN; [6]Department of Medicine, Vanderbilt University, Nashville, TN*

WP 304 **Establishment of Convenient Sample Preparation Method with High Sensitivity and Excellent Reproducibility in Mass Spectrometry Imaging of Endogenous Primary Metabolites**; Tomomi Ichinose[1]; Fusa Murayama[1]; Takanori Ishii[1]; Chihiro Kawano[1]; Ayaka Murayama[1]; Akiko Miki[1]; Yoshinori Fujimura[1]; Yuzo Yamazaki[2]; Hiroyuki Wariishi[1]; Daisuke Miura[1]; *[1]Kyushu University, Fukuoka, Japan; [2]Shimadzu Corporation, Kyoto, Japan*

WP 305 **Ketone Based Matrices for Imaging Proteins**; Junhai Yang[1, 2]; Richard M. Caprioli[1, 3]; *[1]Department of Biochemistry, Vanderbilt University, Nashville, TN; [2]The Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [3]Chemistry, Pharmacology and Medicine, the Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN*

WP 306 **Caffeic Acid as a New Matrix for Enhanced Tissue Imaging of High Molecular Weight Proteins by MALDI Mass Spectrometry**; Xiaodong Wang[1]; Huixin He[1]; Liang Qin[1]; Lulu Chen[1]; Yaqin Liu[1]; *[1]Centre for Imaging & Systems Biology, College of Life and Environmental Sciences, Minzu University of China, Beijing, China*

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WP 308 **3D ToF-SIMS Imaging of Cells**; Daniel J. Graham[1]; Lara J. Gamble[1]; *[1]University of Washington Department of Bioengineering, Seattle, WA*

WP 309 **Uranium Bearing Particle Identification using a Fully Convolutional Neural Network and Watershed Segmentation**; Jay Tarolli; *Pacific Northwest National Laboratory, Richland, WA*

WP 310 **Novel Data Analysis Approaches for Mass Spectrometry Imaging Multicenter Studies**; Stefan Frehse[1]; Jan Hendrik Kobarg[1]; Vitaly Kovalev[2]; Fingal Orlando Galashan[1]; Stefan Schiffler[1]; Klaus Steinhorst[1]; Tobias Boskamp[1, 3]; Andrew Palmer[2]; Rohan A. Thakur[4]; Theodore Alexandrov[1, 2, 5]; Dennis Trede[1, 4]; *[1]SCiLS GmbH, Bremen; [2]EMBL, Heidelberg, Heidelberg; [3]University of Bremen, Bremen, Germany; [4]Bruker Daltonik GmbH, Bremen, Germany; [5]University of California, San Diego, CA*

WP 311 **Real-Time Viewing, Classification and 3D Reconstruction for Imaging Mass Spectrometry**; Richard Chapman[1]; Emrys Jones[1]; Csaba Hajdu[2]; Emmy Hoyes[1]; Praveen Harapanahalli[1]; Emmanuelle Claude[1]; Robert Tonge[1]; Steven Pringle[1]; *[1]Waters Corporation, Wilmslow, UK; [2]Waters Research Center, Budapest*

WP 312 **Mass Spectrometry Image Exploration and Annotation with MSiReader**; Kenneth Garrard[1]; Milad Nazari[1]; Mark Bokhart[1]; Måns Ekelöf[1]; Sitora Khodjaniyazova[1]; David C. Muddiman[1]; *[1]North Carolina State University, Raleigh, NC*

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WP 314 **Specter: Deconvolution of Data Independent Acquisition Mass Spectrometry Data by Linear Regression of Acquired Spectra onto Libraries**; Ryan Peckner[1]; Samuel A Myers[1]; Jarrett Egertson[2]; Richard S Johnson[2]; Michael J MacCoss[2]; Jacob D Jaffe[1]; *[1]Broad Institute, Cambridge, Massachusetts; [2]University of Washington, Seattle, WA*

WP 315 **Philosopher: A Data Processing Toolkit for Shotgun Proteomics**; Felipe da Veiga Leprevost[1]; Avinash Kumar Shanmugam[1]; Alexey I. Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI*

WP 316 **Statistical Analysis of UVPD Fragmentation in the Middle-down Size Regime: A Data-Mining Approach**; Jake Rosenberg[1]; Jennifer S Brodbelt[2]; *[1]University of Texas at Austin, Austin, TX; [2]University of Texas at Austin, Austin, TX*

WP 317 **Discriminating Isobaric Phosphopeptides using Data-Independent Acquisition Mass Spectrometry**; Zuofei Yuan[1]; Simone Sidoli[1]; Rina Fujiwara[1]; Katarzyna Kulej[1, 2]; Benjamin A. Garcia[1]; *[1]University of Pennsylvania, Philadelphia, PA; [2]The Children's Hospital of Philadelphia, Philadelphia, PA*

WP 318 **An Ion Library-Free, Data Independent Acquisition Strategy for Vibrio natriegens Proteome Characterization using Deep DIA's DeepSearch Protocol**; William Judson Hervey, IV[1]; Gautam Saxena[2]; Krystine Pimentel[3]; Gary J. Vora[4]; *[1]Center for Bio/Molecular Science & Engineering, Naval Research Laboratory, Washington, DC; [2]DeepDIA, Bethesda, MD; [3]Department of Computer and Electrical Engineering, Florida International University, Miami, FL; [4]Center for Bio/Molecular Science & Engineering, Naval Research Laboratory, Washington, DC*

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WP 321 **Recent Advances in Skyline: Further Improvements in Small Molecule Targets and Ion Mobility**; Brian Pratt[1]; Will Thompson[2]; Erin S Baker[3]; Michael J MacCoss[1]; Brendan MacLean[1]; *[1]University of Washington, Seattle, WA; [2]Duke University, Durham, North Carolina; [3]PNNL, Richland, WA*

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WP 324 **Software to Facilitate Automated Validation of Imaging Mass Spectrometry Annotations of Metabolites with Follow-Up LC-MS/MS Data**; Ivan Protsyuk[1]; Prasad Phapale[1]; Andrew Palmer[1]; Luca Rappez[1]; Theodore Alexandrov[1, 2]; *[1]EMBL, Heidelberg, Baden-Wuerttemberg; [2]Skaggs School of Pharmacy, University of California San Diego, La Jolla, CA*

WP 325 **Metandem: A Novel Online Software Platform for Mass Spectrometry-Based Isobaric Labeling Metabolomics**; Ling Hao[1]; Pingli Wei[1]; Fabao Liu[2]; Jillian Johnson[1]; Amanda Buchberger[1]; W. John Kao[3]; Wei Xu[2]; Lingjun LI[1]; *[1]University of Wisconsin-Madison, Madison, WI; [2]McArdle Laboratory for Cancer Research, UW-Madison, WI; [3]President's Office, the University of Hong Kong, Hong Kong, China*

WP 326 **DeltaMS: A Convenient Tool to Track Isotopologues in GC/LC-MS Data by Stable Isotope Probing (SIP)**; Tim Baumeister[1]; Nico Ueberschaar[2]; Wolfgang Schmidt-Heck[3]; Jan-Frieder Mohr[2]; Michael Deicke[2]; Thomas Wichard[2]; Reinhard Guthke[3]; Georg Pohnert[1, 2]; *[1]Max Planck Institute for Chemical Ecology, Max Planck Fellow Group Plankton Community Interaction, Jena, Germany; [2]Friedrich Schiller University Jena, Jena, Germany; [3]Leibniz Institute for Natural Product Research and Infection Biology – Hans Knoell Institute (HKI), Department of Systems Biology and Bioinformatics, Jena, Germany*

WP 327 **Metabolite Annotations for Spectra Not Available in Spectral Library Viain Silicomolecular Networking and Raw Data Spectral Matching**; Ricardo Silva[1]; Alexandria Ongjoco[2]; Pieter C. Dorrestein[3, 4]; *[1]University of California, San Diego, CA; [2]Skaggs School of Pharmacy, University of California San Diego, La Jolla, CA; [3]Skaggs School of Pharmacy, University of California San Diego, San Diego, CA; [4]Department of Pediatrics, University of California San Diego, San Diego, CA*

WP 328 **New Algorithms for Reducing the Rate of False Positive and False Negative Compounds Detected from Mass Spectrometry Metabolomics Data**; Owen Myers[1]; Susan Sumner[2]; Shuzhao Li[3]; Stephen Barnes[4]; Xiuxia Du[1]; *[1]University of North Carolina at Charlotte, Charlotte, NC; [2]University of North Carolina at Chapel Hill, Chapel Hill, NC; [3]Emory University, Atlanta, Georgia; [4]University of Alabama at Birmingham, Birmingham, AL*

WP 329 **MetabVision: A Shiny Based Web Framework for Quality Control (QC), Data Normalization and Visualization in Untargeted Metabolomics**; Tanu Soni[1]; Matthew Hansen[2]; Charles Evans[1, 3]; Sarah Tishkoff[2]; Charles Burant[1, 3]; Thekkelnaycke Rajendiran[1, 4]; *[1]Michigan Regional Comprehensive Metabolomics Resource Core,University of Michigan, Ann Arbor, MI; [2]Departments of Genetics and Biology, University of Pennsylvania, Philadelpha, PA; [3]Department of Internal Medicine, University of Michigan, Ann Arbor, MI; [4]Department of Pathology, University of Michigan, Ann Arbor, MI*

WP 330 **Automatic Pipeline Package for Identification and Normalization of LCMS-Based Untargeted Metabolomics**; Chuan-Yih Yu[1]; Johannes Fahrmann[1]; Eunice Murage[1]; Jennifer Dennison[1]; Samir Hanash[1]; *[1]MD Anderson Cancer Center, Houston, TX*

WP 331 **Identifying Biologically Important Metabolites by Mass Spectrometry-Based Cheminformatics**; Zijuan Lai[1]; Hiroshi Tsugawa[2]; Gert Wohlgemuth[1]; Masanori Arita[2];

Oliver Fiehn[1]; [1]*UC Davis, Davis, CA;* [2]*RIKEN Center for Sustainable Resource Science, Yokohama, Kanagawa*

WP 332 **A Web Service Framework for Interactive Browsing of Metabolomics Data**; Yaroslav Lyutvinskiy[1]; Jeramie Watrous[2]; Mohit Jain[2]; Roland Nilsson[1]; [1]*Karolinska institute, CMM, Stockholm, Sweden;* [2]*UCSD, La Jolla, CA*

WP 333 **Galaxy-Centered Lab Workflows to Organize Metabolomic Analyses**; Arthur C. Eschenlauer[1, 2, 3]; Mark Esler[1, 3]; Jerry D. Cohen[1, 3]; Timothy J. Griffin[2, 4]; Adrian D. Hegeman[1, 3]; [1]*Microbial and Plant Genomics Institute and Dept. of Horticultural Science, University of Minnesota, St. Paul, MN;* [2]*Dept. of Biochemistry, Molecular Biology, and Biophysics, University of Minnesota, Minneapolis, MN;* [3]*University of Minnesota, St. Paul, MN;* [4]*University of Minnesota, Minneapolis, MN*

WP 334 **New and Improved Functionality of a Public Resource, MyCompoundID, for Chemical Isotope Labeling LC-MS Metabolomics**; Hao Li[1]; Shuang Zhao[1]; Xian Luo[1]; Taibo Luo[1]; Guohui Lin[1]; Liang Li[1]; [1]*University of Alberta, Edmonton, AB, Canada*

WP 335 **Artificial Neural Networks based Visual Data Mining for Clinical and Metabolomic Data**; Kasun Amarasinghe[1]; Urszula Osinska Warncke[2]; Naren Gajenthra Kumar[1]; Daniel Contaifer[1]; Milos Manic[1]; Dayanjan S Wijesinghe[1]; [1]*Virginia Commonwealth University, Richmond, VA;* [2]*Virginia Commonwealth University, Richmond, VA*

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WP 337 **Guiding Ions with a Quadrupole Operated at Elevated Pressure**; Wen-Ping Peng[1]; Zhuoer Xie[2]; Adam Hollerbach[2]; Dalton T Snyder[2]; Graham Cooks[2]; [1]*National Dong Hwa University, Shoufeng, Taiwan;* [2]*Purdue University, West Lafayette, IN*

WP 338 **Preclinical Pharmacokinetics Study Using Miniature MS System and Culex Automatic Blood Sampler**; Fan Pu[1]; Wenpeng Zhang[2]; Yong Liu[3]; Kevin Bateman[4]; Roy Helmy[3]; Zheng Ouyang[1, 2, 5]; [1]*Department of Chemistry, Purdue University, West Lafayette, IN;* [2]*Weldon School of Biomedical Engineering, Purdue University, West Lafayette, Indiana;* [3]*Merck Research Laboratories, Rahway, NJ;* [4]*Pharmacokinetics, Pharmacodynamics and Drug Metabolism, Merck Research Laboratories, Merck & Co., Inc., West Point, PA;* [5]*Department of Precision Instrument, Tsinghua University, Beijing, China*

WP 339 **Comparison of Canine Sniffing Capability with Portable Mass Spectrometry**; Stamatios Giannoukos[1]; Boris Brkić[1]; Stephen Taylor[1]; [1]*Department of Electrical Engineering and Electronics University Of Liverpool, Liverpool, UK*

WP 340 **Use of a Hexapole Ion Guide in a Miniature, Low Power LC-MS Interface: The Power vs. Performance Tradeoff**; Adrian Southard[1]; Stephanie A Getty[2]; Jerome P Ferrance[3]; Jamie E Elsila[2]; Manuel A Balvin[2]; Carl A Kotecki[2]; [1]*Universities Space Research Association, Columbia, MD;* [2]*NASA Goddard Space Flight Center, Greenbelt, MD;* [3]*J2F Engineering, Charlottesville, VA*

WP 341 **Optimization of Multiple Frequency Waveforms for Ion Isolation and Ion Ejection From a Linear Ion Trap MS for Planetory Exploration**; Dalton Synder[1]; Desmond A. Kaplan[2]; Ryan M Danell[3]; Veronica T. Pinnick[4]; Friso van Amerom[5]; Andrej Grubisic[4]; Paul R Mahaffy[4]; William B. Brinkerhoff[4]; Graham Cooks[1]; [1]*Purdue University, West lafayette, Indiana;* [2]*KapScience LLC, Tewksbury, MA;* [3]*Danell Consulting, Greenville, NC;* [4]*NASA GSFC, Greenbelt, MD;* [5]*Mini-Mass Consulting, Inc., Hyattsville, MD*

WP 342 **A Miniature Mass Spectrometer with a Miniature Ion Funnel**; Yanbing Zhai[1]; Xiaohua Zhang[2]; Wei Xu[1]; [1]*Beijing Institute of Technology, Haidian District, Beijing;* [2]*Anyeep Instrumentation Company, Suzhou, China*

WP 343 **Optimization of the PerkinElmer Torion T-9 Portable GC/MS for Common Field Analyses**; Joshua Wilhide[1]; Ian W Shaffer[1]; Margaret E LaCourse[1]; William R LaCourse[1]; [1]*University of Maryland Baltimore County, Baltimore, MD*

WP 344 **Characterization of a Highly Compact Linear Ion Trap Mass Spectrometer (LITMS)**; Friso H.W. Van Amerom[1]; Ryan M Danell[2]; Xiang Li[3]; Andrej Grubisic[4]; Veronica T. Pinnick[5]; Ricardo D. Arevalo[5]; Stephanie A. Getty[5]; William B. Brinkerhoff[5]; Paul R Mahaffy[5]; [1]*Mini-Mass Consulting, Inc, Hyattsville, MD;* [2]*Danell Consulting, Greenville, NC;* [3]*University of Maryland Baltimore County, Baltimore, MD;* [4]*University of Maryland, College Park, MD;* [5]*NASA GSFC, Greenbelt, MD*

WP 345 **Development of a Portable 13C Isotope Ratio Measurement Technique with Quadrupole Mass Spectrometry**; David McIntosh[1]; Stomatis Giannokous[1]; Brian Thomas[2]; Tom Fildes[3]; Lynn Smith[4]; Stephen Taylor[1]; [1]*University of Liverpool, Liverpool, Merseyside;* [2]*University of Liverpool, Glenn Heights, TX;* [3]*University of Liverpool, Liverpool, UK;* [4]*Norton Priory, Runcorn, UK*

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WP 347 **Electro-kinetic Assisted Electrospray Ionization for Enhanced Complex Sample Analysis**; Muyi He[1]; Zezhen Zhang[1]; Pan Luo[1]; Jie Hong[1]; Wenjing Zhang[1]; Jianli Liu[1]; Xiaoli Zhang[1]; Wei Xu[1]; [1]*Beijing Institute of Technology, Beijing, Beijing*

WP 348 **Determination of Unbound Urinary Amino Acids Incorporated with Creatinine Normalization by LC-MS/MS Method with CLAM-2000 Online Sample Pre-treatment**; Zhe Sun[1]; Jie Xing[1]; Irene Agatha[2]; Daisuke Kawakami[3]; Zhaoqi Zhan[1]; [1]*Application Development & Support Centre, Shimadzu (Asia Pacific) Pte Ltd., Singapore, Singapore;* [2]*School of Physical and Mathematical Science, Nanyang Technical University, Singapore, Singapore;* [3]*Clinical & Biotechnology Business Unit, Shimadzu Corporation, Kyoto, Japan*

WP 349 **Compression Ratio Ion Mobility Programming (CRIMP) in Structures for Lossless Ion Manipulations (SLIM)**; Sandilya Garimella[1]; Yehia M Ibrahim[1]; Ahmed M Hamid[1]; Liulin Deng[1]; Ian K Webb[1]; Erin S Baker[1]; Richard D. Smith[1]; [1]*Pacific Northwest National Laboratory, Richland, WA*

WP 350 **Chaotic Motion of Single Ions in a Toroidal Ion Trap Mass Analyzer**; Ailin Li[1]; Jessica M. Higgs[1]; Daniel E. Austin[1]; [1]*Brigham Young University, Provo, UT*

WP 351 **A Computational Study to Optimize Transfer and Soft-Landing of ESI Particles at Low Pressure on Nano-Optomechanical Sensors**; Diamantis Kounadis[1]; Alexander Lekkas[1]; Loukas Mavrikas[1]; Athanasios Zacharos[1]; Dimitris Papanastasiou[2]; Ioannis Nikolos[3]; Oscar Malvar[4]; Monsterrat Calleja[4]; Javier Tamayo[4]; [1]*Fasmatech Science & Technology, Athens, Greece;* [2]*Fasmatech, Athens,*

Attiki; [3]School of Production Engineering & Management, Technical University of Crete, Crete, Greece; [4]Institute of Microelectronics of Madrid, Tres Cantos, Spain

WP 352 **Development of a Compact Microwave Driven ICP Atom Source for Hydrogen Attachment/Abstraction Dissociation (HAD) of Tandem Mass Spectrometry**; Yuji Shimabukuro[1]; Hidenori Takahashi[2]; Shinichi Iwamoto[2]; Koichi Tanaka[2]; Motoi Wada[1]; *[1]Doshisha University, Kyotanabe, Japan; [2]Shimadzu Corporation, Kyoto*

WP 353 **A Novel Platform of On-line Sample Pre-treatment and LC/MS/MS Analysis for Screening and Quantitation of Illicit Drugs in Urine**; Shao Hua Chia[1]; Zhi Wei Edwin Ting[1]; Daisuke Kawakami[2]; Jie Xing[1]; Zhaoqi Zhan[1]; *[1]Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore; [2]Shimadzu Corporation, Kyoto, Japan*

WP 354 **Gas Assisted Ion Ejection (GAIE) Technique Enables Simultaneous Particle Mass and Size Measurement in a Single Quadrupole Ion Trap Cell**; Caiqiao Xiong[1]; Zongxiu Nie[1]; *[1]Institute of Chemistry, Chinese Academy of Sciences, Beijing, China*

WP 355 **Flavors, Odors, and Contaminants in Alcoholic Beverages using Vacuum Assisted Sorbent Extraction (VASE) and GC/MS Analysis**; Victoria Noad[1]; Daniel B Cardin[1]; *[1]Entech Instruments, Simi Valley, CA*

WP 356 **Importance of Metal Oxide Dissociation in the Liquid Sampling-Atmospheric Pressure Glow Discharge / Orbitrap System for Isotope Ratio Measurements**; Edward Hoegg[1]; Kenneth Marcus[1]; *[1]Clemson University, Clemson, SC*

WP 357 **A "Brick Ion Trap Mass Spectrometer" Driven by a Frequency Scanning Technique**; Ting Jiang[1]; Tang Yang[1]; Hongjia Zhang[2]; Yanbing Zhai[1]; Wei Xu[1]; Dayu Li[2]; Wei Xu[1]; *[1]Beijing Institute of Technology, Haidian District, Beijing; [2]Northeastern University, Shengyang, China*

WP 358 **High-Sensitivity and Simultaneous Analysis of Psychoactive Drugs using LC-MS/MS with Full-Automated Pretreatment System**; Daisuke Kawakami[1]; Toshikazu Minohata[1]; Sihoko Nakano[2]; Noriaki Shima[2]; Akihiro Miki[2]; Munehiro Katagi[2]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Osaka Prefectural Police, Osaka, Japan*

WP 359 **New Digital Mass Scanning Techniques without Dipolar Auxiliary Waveforms**; Katherine G. E. Donahoe[1]; Ashley Marie Moon[1]; Zachary Philip Gotlib[1]; Nathan Michael Hoffman[1]; Peter T. A. Reilly[2]; *[1]Washington State University, Pullman, WA; [2]Washington State University, Pullman, WA*

WP 360 **Supercritical Fluid Chromatography Coupled to Electron Ionization Mass Spectrometry: Development of a New System**; Francesca Rigano[1]; Luigi Mondello[1, 2, 3]; *[1]Chromaleont s.r.l., Messina, Italy; [2]Dipartimento di Scienze Chimiche, Biologiche, Farmaceutiche ed Ambientali, University of Messina, Messina, Italy; [3]Unit of Food Science and Nutrition, Department of Medicine, University Campus Bio-Medico of Rome, Roma, Italy*

WP 361 **Rapid FAIMS Inside the Mass Spectrometry Envelope: Exploring Ion Mobility Separations in the Extreme-Field Region**; Alexandre Shvartsburg[1]; Andrew Entwistle[2]; Roch Andrzejewski[2]; Anisha Harris[2]; Roger Giles[2]; *[1]Wichita State University, Wichita, KS; [2]Shimadzu Research Laboratory Europe, Manchester, UK*

WP 362 **On-line Atomic Force Microscope Tip-Enhanced Laser Ablation Mass Spectrometry**; Md Amir Hossen[1]; Bijay Banstola[1]; Fan Cao[1]; Kermit K. Murray[1]; *[1]Louisiana State University, Baton Rouge, LA*

WP 363 **Development of Simultaneous, Quantitative Elemental and Molecular Chemical Imaging Via Optical and Mass Spectrometries**; Jake T. Shelley[1]; Sunil Badal[1]; Montwaun D. Young[1]; Brian T. Molnar[1]; Courtney L. Walton[1]; Garett M. MacLean[1]; *[1]Department of Chemistry and Chemical Biology, Rensselaer Polytechnic Institute, Troy, NY*

WP 364 **How Far can we Challenge the Fundamentals? A Compact, Polygonal Collision Cell**; Felician Muntean[1]; Stephen Zanon[1]; *[1]Bruker Daltonics, Billerica, MA*

WP 365 **A Single Stage Dual Ion Funnel Device for the Transmission of a Full Mass Range of Ions**; Benjamin E. Draper[1]; Staci N. Anthony[1]; Martin F. Jarrold[1]; *[1]Indiana University, Bloomington, IN*

WP 366 **Electrospray Ionization Zoom Time-of-Flight Mass Spectrometry**; Christopher Brais[1]; Jonas Metternich[2]; Steven Ray[1]; *[1]University at Buffalo, Buffalo, NY; [2]University of Muenster, Institute of Inorganic and Analytical Chemistry, Muenster, Germany*

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WP 368 **Screening of Human Fetal Hippocampus Gangliosides by Ion Mobility Mass Spectrometry**; Mirela Sarbu[1, 2]; Željka Vukelić[3]; David E Clemmer[4]; Alina D Zamfir[1, 2]; *[1]National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, Romania; [2]"Aurel Vlaicu" University of Arad, Arad, Romania; [3]Department of Chemistry and Biochemistry, University of Zagreb Medical School, Zagreb, Croatia; [4]Indiana University, Bloomington, IN*

WP 369 **Separation of Isomeric Sphingosines using Trapped Ion Mobility QTOF-MS**; Matt Willetts[1]; Dirk Wunderlich[2]; Verena Tellstroem[2]; *[1]Bruker Daltonics, Billerica, MA; [2]Bruker Daltonik GmbH, Bremen, Germany*

WP 370 **Improved Metabolomics Analysis using Isotopic Ratio Outlier Analysis (IROA) with Ion Mobility-Mass Spectrometry**; Robin H.J. Kemperman[1]; Chris W.W. Beecher[1, 2]; Richard A. Yost[1]; *[1]University of Florida, Gainesville, FL; [2]IROA Technologies, Gainesville, FL*

WP 371 **Improved Sensitivity for Shotgun Proteomics on a Novel Trapped Ion Mobility Spectrometry (TIMS) – Quadrupole Time-of-Flight (QTOF) Instrument**; Scarlet Beck[1]; Heiner Koch[1]; Florian Meier[1]; Markus Lubeck[2]; Stephanie Kaspar-Schoenefeld[2]; Niels Goedecke[2]; Oliver Raether[2]; Juergen Cox[1]; Matthias Mann[1]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany; [2]Bruker Daltonik GmbH, Bremen, Germany*

WP 372 **Optimizing Sample Introduction for Quantitation of 25-Hydroxyvitamin D in Human Serum using Liquid Chromatography/Ion Mobility/Mass Spectrometry**; Jiajun Lei[1]; Nicholas R. Oranzi[1]; Richard A. Yost[1]; *[1]University of Florida, Gainesville, FL*

WP 373 **Control of Gas-Phase Conformation of 25-Hydroxyvitamin D3 and 3-epi-25hydroxyvitamin D3 for Simultaneous Quantitation using Ion Mobility Mass Spectrometry**; Nicholas Oranzi[1]; Christopher D Chouinard[1]; Richard A. Yost[1]; *[1]University of Florida, Gainesville, FL*

WP 374 **High Resolution Trapped Ion Mobility Mass Spectrometry Analysis of Pharmaceutical Intermediate products**; Qinghe Wang[1]; Keyu Zhou[1]; Jing Lu[2]; Kefei Wang[1]; *[1]Bruker Daltonics, Shanghai, China; [2]Bruker Daltonics, Beijing, China*

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WP 450 **Relative Isotopic Abundance on Orbitrap Fusion: input of Accurate 13C Measurement and 18O/13C2 Separation and Measurements for Annotation in Metabolomics**; Pierre Barbier Saint Hilaire[1]; Benoit Colsch[1]; Christophe Junot[1]; François Fenaille[1]; *[1]CEA, iBiTecS, SPI, Laboratoire d'Etude du Métabolisme des Médicaments, MetaboHUB-Paris, Université Paris Saclay, Gif-sur-Yvette cedex, France*

WP 451 **Into the Unknowns - New Libraries of Recurrent Unidentified Mass Spectra from Biological Materials**; John M. Halket[1]; Anna Caldwell[1]; Wm. Gary Mallard[2]; Nirina Andriamaharavo[2]; Stephen E Stein[2]; *[1]King's College London, London, London; [2]NIST, Gaithersburg, MD*

WP 452 **A High-Resolution Orbitrap GC-MS Spectral Library for Discovery Metabolomics**; Matthew J. P. Rush[1]; Kyle J. Connors[1]; Nicholas W. Kwiecien[1]; Edna A. Trujillo[1]; Jason D. Russell[2]; Michael S. Westphall[1]; Joshua J. Coon[1]; *[1]University of Wisconsin - Madison Department of Chemistry, Madison, WI; [2]Morgridge Institute for Research, Madison, WI*

WP 453 **Evaluation and Application of Lysimeters for Untargeted Soil Solution Analytics and Marker Identification**; Nico Ueberschaar[1]; Katharina Lehmann[1]; Andreas Schmalwasser[1]; Stefanie Meyer[1]; Beate Michalzik[1]; Kai Uwe Totsche[1]; Georg Pohnert[1]; *[1]Friedrich Schiller University Jena, Jena, Germany*

WP 454 **Novel UHPLC-timsTOFMS/MS and UHPLC-MS-SPE-NMR Tools for Higher-throughput, Confident Metabolite Identifications and to Address the Number One Grand Challenge of Metabolomics**; Lloyd W. Sumner[1]; Feng Qiu[2]; Daniel Wherritt[3]; Zhentian Lei[2]; Aiko Barsch[4]; Sven Meyer[4]; *[1]The University of Missouri at Columbia, Columbia, MO; [2]University of Missouri, Columbia, MO; [3]University of Texas at San Antonio, San Antonio, TX; [4]Bruker Daltonics, Bremen, Germany*

WP 455 **Just How Many Unknowns are there in a Metabolomics Data Set? Really?**; Chris Beecher[1]; Timothy J. Garrett[2]; Casey A. Chamberlain[2]; Joy D. Guingab[2]; Richard A. Yost[2]; Alexander Raskind[3]; Felice de Jong[4]; *[1]IROA Technologies, Gainesville, FL; [2]University of Florida, Gainesville, FL; [3]University of Michigan Medical School, Ann Arbor, MI; [4]IROA Technologies, Gainesville, FL*

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WP 458 **Comprehensive Statistical Analysis of the Largest High Resolution Small Molecule ESI/APCI Library as Condition for Confident Compound ID**; Michal Raab[1]; Juraj Lutisan[1]; Milos Suchy[1]; Robert Mistrik[1]; *[1]HighChem, Bratislava, Slovakia*

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WP 470 **Simultaneous and Comprehensive Determination of Tryptophan and its Catabolites in Mouse Tissues by Polarity Switching UHPLC-MRM-MS**; Guan-yuan Chen[1]; Wei Zhong[1]; Zhanxiang Zhou[1, 2]; Qibin Zhang[1, 3]; *[1]Center for Translational Biomedical Research, University of North Carolina at Greensboro, Kannapolis, NC; [2]Department of Nutrition, University of North Carolina at Greensboro, Greensboro, NC; [3]Department of Chemistry & Biochemistry, University of North Carolina at Greensboro, Greensboro, NC*

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WP 474 **Quantification of polyamines and Urea Cycle Metabolites in Biological Samples by HILIC-MS**; Judy Baek[1]; Stefanie Wernisch[1]; Yun Jin Sin[2]; Jaeman Byun[1]; Subramaniam Pennathur[1]; *[1]University of Michigan Medical Center, Ann Arbor, MI; [2]University of Michigan, Ann Arbor, MI*

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WP 485 **Distinct Proteome Remodeling of Industrial Saccharomyces Cerevisiae in Response to Prolonged Thermal Stress or Transient Heat Shock**; Weidi Xiao[1]; Xiaoxiao Duan[1]; Yuping Lin[2]; Qinchen Cao[2]; Qinhong Wang[2]; Wenqing Shui[2, 3]; *[1]College of Life Sciences, Nankai University, Tianjin, China; [2]Tianjin Institute of Industrial Biotechnology, Chinese Academy of Sciences, Tianjin, Tianjin; [3]iHuman Institute, ShanghaiTech University, Shanghai, China*

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WP 487 **Oral Microbiota in Down Syndrome Individuals: Identification by MALDI-Biotyper**; Rafael Celestino Souza[1, 2]; Levy Anderson Alves[1, 3, 4]; Meriellen Dias[2, 4]; Fausto Medeiros Mendes[1]; Ana Lidia Ciamponi[1]; Maria Anita Mendes[2, 4]; *[1]Dental School of USP, São Paulo, Brazil; [2]Universidade de São Paulo - USP, Sao Paulo, South America; [3]Guarulhos University, Guarulhos, Brazil; [4]Dempster Mass Lab- POLI- USP, Sao Paulo, Brazil*

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WP 492 **MycoDB: New Spectral Database for Identification of Mycobacterium species by MALDI-TOF MS**; Kyu H. Park[1]; Jae-Seok Kim[2]; Sue Shin[3]; Taek Soo Kim[3]; Eun-Kyeong Choi[1]; Yongha In[1]; Hyung Soon Park[1]; Yangsun Kim[1]; *[1]ASTA, Suwon, South Korea; [2]Department of Laboratory Medicine, Hallym University College of Medicine, Chuncheon, South Korea; [3]Seoul National University College of Medicine, Jongno-gu, South Korea*

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WP 495 **Profiling of Small Molecules for the Discrimination of Bacillus cereus and Bacillus thuringiensis by MALDI-TOF MS** ; Yangsun Kim[1]; Miyoung Ha[2]; Eun-Kyeong Choi[3]; Yongha In[3]; *[1]ASTA, Suwon, Gyeonggi; [2]Nonghyup Food Research Institute, Suwon-si, South Korea; [3]ASTA, Suwon, South Korea*

WP 496 **Proteomic Characterization of Particle Content and Infectious Cycle of Pandoraviruses, A Recently Discovered Family of Giant Viruses.**; Laure Beucher[1]; Elisabeth Fabre[2]; Lucid Belmudes[1]; Matthieu Legendre[2]; Anne-Marie Hesse[1]; Olivier Poirot[2]; Sandra Jeudy[2]; Christophe Bruley[1]; Jean-Michel Claverie[2]; Chantal Abergel[2]; Yohann Couté[1]; *[1]EDyP UMR1038 Inserm/CEA/UGA, Grenoble, France; [2]Information Génomique & Structurale, Unité Mixte de Recherche 7256 (Institut de Microbiologie de la Méditerranée, FR3479) Centre National de la Recherche Scientifique, Marseille cedex 9, France*

WP 497 **Identification of Common Food-Borne Pathogens at Species and Sub-Species Level by LC-MS/MS**; Shu-Hua Chen[1]; Christine H. Parker[1]; Timothy R. Croley[1]; Melinda A. McFarland[1]; *[1]U.S. Food and Drug Administration, College Park, MD*

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WP 499 **Nicotine-Induced Proteome of Arthrobacter nicotinovorans pAO1+**; Marius Mihasan[1, 2]; Cornelia Babii[1]; Roshanak Aslebagh[2]; Costel C. Darie[2]; *[1]Biochemistry and Molecular Biology Laboratory, Faculty of Biology, Alexandru Ioan Cuza University, Iasi, Romania; [2]Biochemistry & Proteomics Group, Department of Chemistry & Biomolecular Science, Clarkson University, Potsdam, NY*

WP 500 **Quantitative Proteome Analyses of Diverse Mycobacterium Tuberculosis Clinical Isolate Strains by SWATH-MS**; Ben Collins[1]; Amir Banaei-Esfahani[1, 2]; Olga T Schubert[1, 3]; Andrej Trauner[4]; Sonia Borrell[4]; Mireia Coscolla[4]; Sebastien Gagneux[4]; Ruedi Aebersold[1, 5]; *[1]Department of Biology, Institute of Molecular Systems Biology, ETH Zurich, Zurich, Switzerland; [2]PhD Program in Systems Biology, University of Zurich and ETH Zurich, Zurich, Switzerland; [3]Present address: Departments of Human Genetics, University of California, Los Angeles, CA; [4]Department of Medical Parasitology and Infection Biology, Swiss Tropical and Public Health Institute, Basel, Switzerland; [5]Faculty of Science, University of Zurich, Zurich, Switzerland*

WP 501 **Mass Spectrometry Imaging and Electron Microscopy of Drip-Flow Generated Biofilm Induced Corrosion**; Joseph F. Ellis[1]; Bin Li[1]; Sage J. B. Dunham[1]; Justin D. Lange[2]; Clint M Arnett[2]; Jonathan V Sweedler[1]; *[1]Department of Chemistry and the Beckman Institute, University of Illinois at Urbana−Champaign, Urbana, IL; [2]Engineer Research and Development Center-Construction Engineering Research Laboratory (ERDC-CERL), Champaign, IL*

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WP 511 **Use of Mass Spectrometry in the Hunt for Novel Lytic Bacteriophage Active Against Pathogenic E. coli.**; Leslie Harden[1]; Yen-Te Liao[1]; Anna Bates[1]; Vivian Wu[1]; *[1]USDA/ WRRC, Albany, CA*

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WP 514 **Characterization of Polystyrene and Silica Beads in Submicrometer Range using Flow Filed-Flow Fractionation and Flow Cytometry**; Zhishang Hu[1]; Chen Ye[2]; Wei Mi[3]; Hongmei Li[3]; Haiying Hang[2]; *[1]NIM, China, Beijing, Beijing; [2]IBP, CAS, China, Beijing, China; [3]NIM, China, Beijing, China*

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WP 517 **Dynamic pH Junction Based Capillary Zone Electrophoresis-Mass Spectrometry with Half-a-Microliter Loading Capacity and 140-min Separation Window for Bottom-Up Proteomics**; Daoyang Chen[1]; Liangliang Sun[1]; Xiaojing Shen[1]; *[1]Michigan State University, East Lansing, MI*

WP 518 **Fast Chip-CEMS for Characterization of Protein/PTM Changes**; Deborah R Leon[1]; Kshitij Khatri[1]; Bo Yan[1]; John R Hasserick[1]; Christian Heckendorf[1]; Joseph Zaia[1]; Catherine E. Costello[1]; Mark E. Mccomb[1]; *[1]Boston University School of Medicine, Boston, MA*

WP 519 **Capillary Electrophoresis and Ion Mobility Coupled to Mass Spectrometry as Complementary Tools for Cysteine Connectivity Identification in Peptides**; Cedric Delvaux[1]; Philippe Massonnet[1]; Christopher Kune[1]; Jean R. N. Haler[1]; Grégory Upert[2]; Gilles Mourier[2]; Nicolas Gilles[2]; Loïc Quinton[1]; Johann Far[1]; Edwin De Pauw[1]; *[1]Mass Spectrometry Laboratory, University of Liège, Liège, Belgium; [2]Commissariat à l'Energie Atomique et aux Energies Alternatives, iBiTec-S, SPI, LEMM, Gif Sur Yvette, France*

WP 520 **Characterization of Anions by Microchip Capillary Electrophoresis-Negative Electrospray Ionization-Mass Spectrometry**; Justin M. Godinho[1]; J. Michael Ramsey[1]; *[1]The University of North Carolina at Chapel Hill, Chapel Hill, NC*

WP 521 **A Fully Automated Microchip Capillary Electrophoresis-ESI-MS System for High Throughput Analysis of Metabolites, Peptides, and Intact Proteins**; Joshua P. Guerrette[1]; Erin A. Redman[1]; Michael P Goodwin[2]; J. Scott Mellors[1]; *[1]908 Devices, Inc., Carrboro, NC; [2]908 Devices Inc., Boston, MA*

WP 522 **Ionic Liquid-Based Slug-Flow Microextraction for Ambient Ionization Mass Spectrometry**; Yueguang Lv[1, 2]; Qiang Ma[1]; *[1]Chinese Academy of Inspection and Quarantine, Beijing, China; [2]University of Chinese Academy of Sciences, Beijing, China*

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WP 523 **Biomolecular Interactions on Cheese Rinds: Pseudomonas vs. Candida**; Shilpa Kolachina[1]; Emily Pierce[2]; Rachel J. Dutton[2]; Laura M. Sanchez[3]; *[1]College of Engineering, University of Illinois at Chicago, Chicago, IL; [2]Division of Biological Sciences, University of California San Diego,, San Diego, CA; [3]Department of Medicinal Chemistry and Pharmacognosy, University of Illinois at Chicago, Chicago, IL*

WP 524 **Natural Product Bioactive Peptide Discovery using PepSAVI-MS**; Christine L. Kirkpatrick[1]; Nicole C. Parsley[2]; Leslie M. Hicks[2]; *[1], Chapel Hill, NC; [2]UNC-Chapel Hill, Chapel Hill, NC*

WP 525 **Valve Based 2D-UHPLC/QTOF MS Solution for Exploring Natural Products** ; Guoqiang Liu[1]; Yue Song[1]; Bo Chen[1]; Shan-An Chan[2]; *[1]Agilent Technology, Shanghai, China; [2]Agilent Technology, Taipei, Taiwan*

WP 526 **MagMASS as a Drug Discovery Platform - Screening Actinobacteria for Novel Ligands of Fructose-1,6-Bisphosphatase**; Michael D Rush[1]; Brian T Murphy[1]; Richard B. van Breemen[1]; *[1]University of Illinois at Chicago College of Pharmacy, Chicago, IL*

WP 527 **Quantification of Aconite Alkaloids in Chinese Proprietary Medicines by LC-ESI-MS/MS and its Application in Product Safety Evaluation**; Ge Xiaowei[1]; Yun Zeng[1]; Chee-Leong Kee[1]; Min-Yong Low[1]; *[1]Health Sciences Authority, Singapore, Singapore*

WP 528 **MS-based Screening of Licorice Extracts for Chemopreventive Agents that Covalently Modify Keap1 Protein, A Regulator of the Antioxidant Response element**; Lingyi Huang[1]; Amanda E. Lee[1]; Charlotte Simmler[1]; Yang Yu[1]; Shao-Nong Chen[1]; Guido F. Pauli[1]; Richard B. van Breemen[1]; *[1]University of Illinois at Chicago College of Pharmacy, Chicago, IL*

WP 529 **Characterization of the Secondary Metabolome of Penicillium using Isotopic Labeling and HPLC-HRMS**; Thaïs Hautbergue[1, 2]; Olivier Puel[1]; Souria Tadrist[1]; Laurent Debrauwer[1, 2]; Isabelle P. Oswald[1]; Emilien L. Jamin[1, 2]; *[1]Toxalim (Research Centre in Food Toxicology), Toulouse University, INRA, ENVT, INP-Purpan, UPS, Toulouse, France; [2]INRA, Platform MetaboHub-MetaToul-AXIOM, Toulouse, France*

WP 530 **Rapid Glucosinolate Detection and Identification using Accurate Mass MS-MS**; Mark Berhow; *USDA, ARS, NCAUR, Peoria, IL*

WP 531 **Qualitative and Quantitative Determination of Cannabinoid Profiles and Potency in Hemp Oil using LC-UV-MS**; Mike Adams[1]; Annette Roth[1]; Sue D'Antonio[2]; Guannan Li[2]; John Palmer[2]; Jamie Dougherty[2]; Anthony Macherone[2, 3]; *[1]CWC Labs, Austin, TX; [2]Agilent Technologies Inc., Santa Clara, CA; [3]Johns Hopkins University School of Medicine, Baltimore, MD*

WP 532 **Metabolite Profiling and Localization of Triterpene Glycosides from the Sea Cucumber Eupentacta Fraudatrix**; Roman S. Popov[1]; Pavel S. Dmitrenok[1]; *[1]: G.B. Elyakov Pacific Institute of Bioorganic Chemistry, Far Eastern Branch of the Russian Academy of Sciences, Vladivostok, Russia*

WP 533 **Tracking the Bryostatin β-branching Type II Polyketide Synthase "In-action" via Optimized Digestion and nLC-FTMS**; Phillip J. McClory[1]; Samuel T. Slocum[2]; Vikram V. Shende[1]; David H. Sherman[1]; Kristina Hakansson[1]; *[1]University of Michigan, Ann Arbor, MI; [2]University of Michigan Medical School, Ann Arbor, MI*

WP 534 **Using Multiple Complimentary Analytical Platforms to Investigate Synergistic Relationships between Bioactive Compounds in Natural Herbal Extracts**; Phillip Kirkland[1]; Alex Yiannikouris[1]; *[1]Alltech, Inc., Nicholasville, KY*

WP 535 **Identification of the Surface Abiotic Degradation Products of UK-2A and the Biological Activity Relevance**; Quanbo Xiong[1]; Kyung Myung[2]; Chenglin Yao[2]; Paul R. Graupner[2]; Yelena Adelfinskaya[2]; John F. Daeuble[2]; Meyer T. Stacy[2]; Zachary Buchan[2]; Nick X. Wang[2]; Kevin G. Meyer[2]; *[1]Dow AgroSciences, Indianapolis, IN; [2]Dow AgroSciences, Indianapolis, IN*

WP 536 **Approaches to Monitor Reactions of Small Molecules with Cell Membranes and Peptides with Cell Membranes by Liquid Chromatography-Mass Spectrometry**; Hannah M Britt[1]; Vian S Ismail[1]; John M Sanderson[1]; Jackie Mosely[1]; *[1]Department of Chemistry, Durham University, Durham, UK*

WP 537 **Discovering Metabolites Using Molecular networking: Case Studies for Biomarker Discovery from Cystic Fibrosis Sputa and Patient Metabolism of Antihypertensive Drugs**; Natalie Castellana[1]; Anand Patel[1]; *[1]Digital Proteomics, LLC., La Jolla, CA*

WP 538 **Characterization of Polyphenol Derivatives in Pinus Armandii Franchet by Solvent-Compensation Liquid Chromatography Applied with Energy-Resolved Mass Spectrometry**; Pai-Chi Syue[1]; Ya-Zhu Zhang[1]; Mai-Su Lin[1]; Kuo-Lung Ku[1]; *[1]National Chiayi University, Chiayi City, Taiwan*

WP 539 **The Features of the Fragmentations of Rare Starfish Cyclic Steroidal Glycosides in the ESI MS/MS Spectra**; Pavel Dmitrenok; *G.B. Elyakov Pacific Institute of Bioorganic Chemistry, Far Eastern Branch of the Russian Academy of Sciences, Vladivostok, Russia*

WP 540 **A Rapid Method for Evaluation the Quality of Tea through Screening the Secondary Metabolites by Screen-Printed Carbon Electrode Spray**; Che-I Liao[1]; Zong-Yi Wu[1]; Kuo-Lung Ku[1]; *[1]National Chiayi University, Chiayi City, Taiwan*

WP 541 **A Tale of Two Cultures: Co-culturing of a Fungus with MRSA**; Diana Kao[1]; Huzefa A. Raja[1]; Daniel A. Todd[1]; Nadja B. Cech[1]; Nicholas H. Oberlies[1]; *[1]University of North Carolina at Greensboro, Greensboro, NC*

WP 542 **Cordyceps: A Biologically Complex Age-Old Fungal Medicine**; Chad C. Nelson[1]; Krishna Parsawar[2]; Douglas N. Stevenson[1]; *[1]Nu Skin Enterprises, Provo, UT; [2]University of Utah, Salt Lake City, UT*

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WP 544 **Probing the Stoichiometry and Binding Interfaces of Retroviral RNA-Peptide Complexes by Native Top-Down Mass Spectrometry**; Eva-Maria Schneeberger[1]; Kathrin Breuker[1]; *[1]University of Innsbruck, Innsbruck, Tirol*

WP 545 **HRAM-LC/MS3 DNA Adductomic Approach, A Comprehensive Methodology to Investigate DNA Damage Induced by Nanomaterials**; Andrea Carra[1]; Silvia Balbo[1]; Tian Qiu[2]; Peter W. Villalta[1]; Taylor Linn[3]; Vivian

Feng[3]; Christy Haynes[2]; *[1]Masonic Cancer Center, University of Minnesota, Minneapolis, MN; [2]University of Minnesota Twin Cities, Chemistry Department, Minneapolis, MN; [3]Augsburg College, Chemistry Department, Minneapolis, MN*

WP 546 **Stoichiometry of HIV-1 Gag Polyprotein-RNA Complexes as Determined by Native Mass Spectrometry**; Samantha H Hinckley[1]; Erik D Olson[1]; Karin Musier-Forsyth[1]; Vicki H. Wysocki[1]; *[1]The Ohio State University, Columbus, OH*

WP 547 **Negative-Ion Mode RNA Top-down Mass Spectrometry for Revealing Interaction Sites within RNA-Protein Complexes**; Kevin M Ileka[1]; Kristina Hakansson[2]; *[1]University of Michigan, Ann Arbor, MI; [2]University of Michigan, Ann Arbor, MI*

WP 548 **Improved Mapping of Eukaryotic mRNA-binding Regions on Proteins using High Resolution Mass Spectrometry**; Meeli Mullari[1]; David Lyon[1]; Lars Juhl Jensen[1]; Michael L Nielsen[1]; *[1]NNF CPR, Copenhagen*

WP 549 **RNA Modification Mapping Using Mass-to-Charge Dependent Collision Energies on a Synapt G2-S**; Peter A. Lobue[1]; Balasubrahmanyam Addepalli[1]; Patrick A. Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH*

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WP 551 **LC/MS Oligonucleotide Mass Fingerprinting (OMF) Enables Rapid Characterization of Critical Quality Attributes in Therapeutic mRNA**; Serenus Hua[1]; Srujan Kumar Gandham[1]; Tao Jiang[1]; Kerry Salandria[1]; Chisom Udengwu[1]; Ipsita Roymoulik[1]; James D. Thompson[1]; *[1]Moderna Therapeutics, Cambridge, MA*

WP 552 **Two-Dimensional Liquid Chromatography-Mass Spectrometry for the Characterization of Oligonucleotide Impurities**; Stilianos G. Roussis[1]; Claus Rentel[1]; *[1]Ionis Pharmaceuticals, Inc., Carlsbad, CA*

WP 553 **LC-MS Based Determination of Pseudouridine at Single Nucleotide Resolution in Mammalian Non-Coding RNAs using a Uridine Synthesis Deficient Cell line**; Yuka Yamaki[1]; Yuko Nobe[1]; Hiroshi Nakayama[2]; Hideaki Ishikawa[3]; Yoshio Yamauchi[1]; Nobuhiro Takahashi[3]; Toshiaki Isobe[1]; Masato Taoka[1]; *[1]Department of Chemistry, Tokyo Metropolitan Univ., Tokyo, Japan; [2]RIKEN Center for Sustainable Resource Science, Wako, Japan; [3]Tokyo University of Agriculture and Technology, Fuchyu, Japan*

WP 554 **Mass Spectrometry and Next Generation Sequencing Analysis of tRNAs from the Pathogenic Fungi Cryptococcus Neoformans**; Mellie Paulines[1]; Andrew Holmes[2]; Todd lowe[2]; Patrick A. Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH; [2]University of California, Santa Cruz, Santa Cruz, CA*

WP 555 **Direct identification of miR-451 from plasma using LC-MS**; Babak Basiri[1]; Michael Bartlett[1]; *[1]University of Georgia, Athens, GA*

WP 556 **Detection and Mapping of Post-Transcriptional tRNA Modifications in the Radioresistant Bacterium Deinococcus radiodurans**; Ruoxia Zhao[1]; Patrick A Limbach[2]; *[1]University of Cincinnati, Cincinnati, OH; [2]University of Cincinnati, Cincinnati, OH*

WP 557 **Using LC/ESI-FTMS to Identify Cellular Damage Products within the RNA of a Radiotrophic Species**; Whitney Houser[1]; Lauren Schultz[1]; Patrick A. Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH*

WP 558 **Rapid Genotyping of Oenanthe Javanica and Cicuta virosa by Polymerase Chain Reaction Followed by Liquid Chromatography/Mass Spectrometry**; Hajime Miyaguchi[1]; Tadashi Yamamuro[1]; Daisuke Watanabe[1]; Hikoto Ohta[1]; *[1]National Research Institute of Police Science, Kashiwa*

WP 559 **LC-MS/MS-based Quantitative Measurement of 8,5′-Cyclopurine-2′-Deoxynucleosides with Small Quantities of DNA**; Yuxiang Cui[1]; Yinsheng Wang[1]; *[1]University of California, Riverside, Riverside, CA*

WP 560 **Nonspecific Versus Specific Binding of Amino Acids and Dipeptides to RNA Probed by Electrospray Ionization and Collisionally Activated Dissociation**; Jovana Vusurovic[1]; Kathrin Breuker[2]; *[1]University of Innsbruck, Innsbruck, Austria; [2]University of Innsbruck, Innsbruck, Austria*

WP 561 **Screening of DNA Adducts Induced by NNK and LPS Combined Exposures via a High Resolution LC-MS3 Adductomic Approach**; Andrea Carra[1]; Peter W. Villalta[1]; Romel P. Dator[1]; Laura Maertens[1]; Fekadu Kassie[1]; Silvia Balbo[1]; *[1]Masonic Cancer Center, University of Minnesota, Minneapolis, MN*

WP 562 **A Novel Approach for Detecting and Quantifying DNA Modification Using NanoLC-MS/MS**; Ranran Wu[1]; Kevin Janssen[1]; Benjamin A. Garcia[1]; *[1]University of Pennsylvania, Philadelphia, PA*

WP 563 **Affinity Selection Mass Spectrometry Enables Small Molecule Ribosome Binding Analysis**; Thomas O'Connell[1]; Justin Stroh[1]; Jason Ramsay[2]; Donna Petersen[1]; Paula Loria[1]; Bruce Maguire[1]; *[1]Pfizer, Groton, CT; [2]Pfizer Inc, St Louis, MO*

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WP 564 **De Novo Sequencing of Peptides Derived from Scorpion Venom**; Meng Li[1]; Yuko P. Y. Lam[1]; Peng Chen[2]; Maria van Agthoven[1]; Qiong Wu[2]; Mark P. Barrow[1]; Hongzheng Fu[2]; Peter B. O'Connor[1]; *[1]University of Warwick, Coventry, UK; [2]Peking University, Beijing, China*

WP 565 **Determination of the Prominent Fragment Ions Formed by Hot Electron Capture Dissociation (HECD) of Doubly-Charged Peptides and Tryptic Phosphopeptides**; Mark J. Raftery; *Bioanalytical Mass Spectrometry, Sydney, NSW*

WP 566 **Paleoproteomic Analysis of Early Pleistocene Fossil Remains**; Enrico Cappellini[1]; Anna Katerina Fotakis[1]; Rosa Rakownikow Jersie-Christensen[2]; David Lyon[2]; José Víctor Moreno Mayar[1]; Maia Bukhsianidze[3]; Christian D. Kelstrup[2]; David Lordkipanidze[3]; Jesper Velgaard Olsen[2]; Eske Willerslev[1]; *[1]Natural History Museum of Denmark, University of Copenhagen, Copenhagen, Denmark; [2]Novo Nordisk Foundation Center for Protein Research, Faculty of Health Sciences, University of Copenhagen, Copenhagen, Denmark; [3]Georgian National Museum, Tbilisi, Georgia*

WP 567 **Expansion of the Brachylophosaurus Canadensis Collagen I Sequence and Additional Evidence for the Preservation of Cretaceous Protein**; Elena R. Schroeter[1]; Caroline J. DeHart[2]; Timothy P. Cleland[3]; Wenxia Zheng[1]; Paul M. Thomas[2]; Neil L Kelleher[2]; Marshall Bern[4]; Mary H. Schweitzer[1]; *[1]North Carolina State University, Raleigh, NC; [2]Northwestern University, Evanston, IL; [3]University of Texas at Austin, Austin, TX; [4]Protein Metrics Inc., San Carlos, CA*

WP 568 **Structural Characterization of Spider PeptidePhα1β Using Mass Spectrometry Based Approaches**; Kelly L. Wormwood[1]; Armand G. Ngounou Wetie[1]; Marcus V. Gomez[2]; Costel C. Darie[1]; *[1]Clarkson University, Potsdam, NY; [2]Institute of Education and Research Santa Casa Belo Horizonte-Laboratory of Toxins, Belo Horizonte, Brazil*

WP 569 **Rapid and Sensitive Phosphoproteomics on a Modified Q Exactive™ HF**; Dorte B. Bekker-Jensen[1]; Christian D. Kelstrup[1]; Tabiwang Arrey[2]; Alexander Hogrebe[1]; Alexander Harder[2]; Jesper V. Olsen[1]; *[1]CPR, University of Copenhagen, Copenhagen, Denmark; [2]Thermo Fisher Scientific, Bremen, Germany*

WP 570 **Low Dispersion Electrochemical Flow Cell for On-Line LC-EC-MS**; Martin Eysberg[1]; Jean-Pierre Chervet[2]; Hendrik-Jan Brouwer[2]; Pablo Sanz de la Torre[2]; *[1]Antec Scientific*

(USA), Boston, MA; [2]Antec Scientific, Zoeterwoude, Netherlands

WP 571 **LC-MS Method to Evaluate Incidence Rate of Protein Sequence Variants in Biopharmaceuticals**; Heather Oakes[1]; Sylwia Jozwiak[1]; Marc Feary[2]; Frances Kenny[1]; Steve Flatman[1]; James Graham[1]; *[1]Lonza Biologics, Slough, Berkshire; [2]Lonza Biologics, Cambridge, UK*

WP 572 **Identification and Localization of Modified Residues in Disulfide-Linked Peptides via CID of Anionic Species**; Alice L. Pilo[1]; Weijuan Tang[1]; *[1]Merck & Co., Inc, Rahway, NJ*

WP 573 **Proteogenomic Analyses of Neoantigen Diversity in Cisplatin-Resistant Ovarian Cancer Cells**; Nicholas W. Bateman[1, 2]; Guisong Wang[1]; Brian L. Hood[1]; Chad A. Hamilton[1, 3]; George L. Maxwell[1, 4]; Thomas P. Conrads[1, 4]; *[1]WHIRC, Annandale, VA; [2]The John P. Murtha Cancer Center, Walter Reed National Military Medical Center, Bethesda, MD; [3]Gynecologic Oncology Service, Walter Reed National Military Medical Center, Bethesda, MD; [4]Inova Schar Cancer Institute, Falls Church, VA*

WP 574 **A Systematic and Quantitative Study on Kinetics of Immobilized Trypsin Based Protein Digestion**; Xiaojing Shen[1]; Daoyang Chen[1]; Liangliang Sun[1]; *[1]Michigan State University, Lansing, MI*

WP 575 **SWATHTM-Data Independent Acquisition Strategies for Ultimate Confidence in Peptide Mapping and Post Translational Modifications quantitation for Biotherapeutics Characterization**; Sibylle Heidelberger[1]; Annu Uppal[2]; *[1]SCIEX, Concord, ON, Canada; [2]Sciex, India, Gurgaon, India*

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WP 577 **Analysis of Amyloid-Beta Isoform Composition in Human Blood Plasma and Platelets**; Anna Bugrova[1]; Maria I. Indeykina[1, 2, 3]; Natalia V. Zakharova[1]; Alexey S Kononikhin[2]; Stanislav I. Pekov[2, 3]; Igor Popov[1, 2]; Sergey A. Kozin[4]; Eugene (Evgeny) Nikolaev[2, 5, 6]; *[1]Emanuel Institute of Biochemical Physics of Russian Academy of Sciences, Moscow, Russia; [2]Moscow Institute of Physics and Technology (State University), Dolgoprudnyj, Russia; [3]Institute for Energy Problems of Chemical Physics of RAS, Moscow, Russia; [4]Engelhardt Institute of Molecular Biology, Moscow, Russia; [5]Skolkovo institute of science and technology, Skolkovo, Russia; [6]Institute of energy problems of chemical physics Russian Academy of Sciences, Moscow, Russia*

WP 578 **Quantitation of Low-Level Peptide Impurities in Certified Reference Materials and Incorporation of Ion Mobility Mass Spectrometry for Conformational Isomer Characterization**; Bradley Stocks[1]; Marie-Pier Thibeault[1]; Juris Meija[1]; Jeremy Melanson[1]; *[1]National Research Council Canada, Ottawa, ON, Canada*

WP 579 **"Shotgun Microdialysis" with LC-MS3 Quantitation for the Screening of BBB Penetration Properties of Peptide-Based Drugs**; Catherine Kramer[1]; Mitchell J. Bartlett[1]; Evan M. Jones[1]; Chris Stagg[1]; Robin Polt[1]; Torsten Falk[1]; Michael L. Heien[1]; *[1]University of Arizona, Tucson, AZ*

WP 580 **Development of a Sensitive Method (pM levels) for a Lipidated Peptide in Rat Plasma Using Hybrid Immuno-affinity Purification with LC-MS/MS** ; Cynthia M. Chavez-Eng[1]; Dina Goykhman[1]; Yifan Song[1]; *[1]Merck & Co., Inc, Kenilworth, NJ*

WP 581 **Improved Solid-Phase Extraction Protocol and Sensitive Quantification of Six Microcystins in Water using an HPLC-orbitrap Mass Spectrometry System**; Dilrukshika S. W. Palagama[1]; Raymond E West III[2]; Dragan Isailovic[2]; *[1]The University of Toledo, Toledo, OH; [2]University of Toledo, Toledo, OH*

WP 582 **The Application of Targeted Proteomics for Investigating Organic Cation Transporter Protein Mediated Drug-Drug Interaction Between Rifampicin and Metformin** ; Katya Govender[1, 2]; John Howard Adamson[2]; Peter Owira[1]; *[1]University of Kwazulu-Natal, Durban, South Africa; [2]Africa Health Research Institute (AHRI), Durban, South Africa*

WP 583 **Development of a PRM Method to Quantify HLA Class I Peptides in Leukemia Cells**; Laura Herring[1, 2]; Sally Hunsucker[3]; Courtney Elliott[3]; Lee Graves[1, 2, 3]; Gianpietro Dotti[3, 4]; Paul Armistead[3, 5]; *[1]Department of Pharmacology, UNC-Chapel Hill, Chapel Hill, NC; [2]UNC Proteomics Core Facility, UNC-Chapel Hill, Chapel Hill, NC; [3]Lineberger Comprehensive Cancer Center, Chapel Hill, NC; [4]Department of Microbiology and Immunology, UNC-Chapel Hill, Chapel Hill, NC; [5]Department of Medicine, UNC-Chapel Hill, Chapel Hill, NC*

WP 584 **Improved Quantification of the Therapeutic Peptide Liraglutide in Human Plasma**; Mark David Platt[1]; Damon I. Papac[1]; *[1]ICON Bioanalytical Laboratories, Clinton, NY*

WP 585 **Comparison of Mass Spectrometric Immunoassay and Magnetic Beads Assay for Quantitation of Peptide in Rat and Dog Plasma with LC/MS/MS**; Ming Wang[1]; Yang Xu[1]; Tonya Jackson[1]; Steven Bucher[1]; Danny Choo[1]; Helengrace Schuck[1]; Xiang Yu[1]; James Schiller[1]; *[1]Pharmacokinetics, Pharmacodynamics and Drug Metabolism, Merck Research Laboratories, Merck & Co., Inc., West Point, PA*

WP 586 **HPLC-QqOrbitrap Analyses Reveal a Significant Reduction of Tachykinin and Opioid Neuropeptides Level in PC1 and PC2 Mutant Mouse Spinal Cords**; Mouna Saidi[1]; Soufiane Kamali[1]; Francis Beaudry[1]; *[1]Université de Montréal, St-Hyacinthe, QC, Canada*

WP 587 **Extraction of MC-LR from Serum and its Quantification by LC-ESI-Orbitrap-MS**; Rachel K Marvin[1]; Dilrukshika S. W. Palagama[1]; David Baliu-Rodriguez[1]; Bruce S Levison[1]; Judy Westrick[2]; David Kennedy[1]; Kenneth Hensley[3]; Dragan Isailovic[1]; *[1]University of Toledo, Toledo, OH; [2]Wayne State University, Detroit, MI; [3]Arkansas College of Osteopathic Medicine, Fort Smith, AR*

WP 588 **Understanding Cellular Drug Response by Measuring Apoptosis Pathway Members using the TOMAHAQ assay**; Robert A. Everley[1]; Kartik Subramanian[1]; John A. Bachman[1]; Brian K Erickson[1]; Alison R. Erickson[1]; Matthew J. Berberich[1]; Christopher M. Rose[2]; Jeffery Knott[3]; Caitlin E. Mills[1]; Yvonne Hua[1]; Mirra Chung[1]; Steven P. Gygi[1]; Peter K. Sorger[1]; *[1]Harvard Medical School, Boston, MA; [2]Genentech, Inc., South San Francisco, CA; [3]Cell Signaling Technologies, Danvers, MA*

WP 589 **A SRM/MRM Based Targeted Proteomics Strategy for Quantification of Potential Biomarkers of TKI Sensitivity in EGFR Mutated Lung Adenocarcinoma**; Shivangi Awasthi[1, 2]; Tapan Maity[1]; Xu Zhang[1]; Benjamin L. Oyler[3]; David R. Goodlett[2]; Udayan Guha[1]; *[1]Thoracic & Gastrointestinal Oncology Branch, CCR, NCI, Bethesda, MD; [2]School of Pharmacy, University of Maryland, Baltimore, MD; [3]Institute of Marine and Environmental Technology, University of Maryland Center for Environmental Science, Baltimore, MD*

WP 590 **Application of MALDI-TOF-MS for Improvement of Quantitative Determination of α- and β-Asp7 Isoforms of amyloid-β Peptide for Alzheimer's Disease Diagnostics**; Stanislav Pekov[1, 2]; Maria Indeykina[2, 3]; Anna Bugrova[3]; Alexey Kononikhin[1, 2, 3, 4]; Igor Popov[1, 2]; Eugene (Evgeny) Nikolaev[1, 2, 5]; *[1]Moscow Institute of Physics and Technology (State University), Dolgoprudnyj, Russia; [2]Institute for Energy Problems of Chemical Physics of RAS, Moscow, Russia; [3]Emanuel Institute of Biochemical Physics of*

Russian Academy of Sciences, Moscow, Russia; [4]Federal State Budget Institution "Research Center for Obstetrics, Gynecology and Perinatology" Ministry of Healthcare of the Russian Federation, Moscow, Russia; [5]Skolkovo institute of science and technology, Moscow Region, Russia

WP 591 **Human Tissue Distribution of Carbonyl Reductase 1 Using Proteomic Approach with LC-MS/MS**; Wenyi Hua[1]; Hui Zhang[1]; Sangwoo Ryu[1]; Xin Yang[1]; Li Di[1]; *[1]Pfizer Inc., Groton, CT*

WP 592 **Targeted Proteogenomics of Outer Membrane Vesicles Mediating Antibiotic Resistance Transfer among the Acinetobacter**; William Judson Hervey, IV[1]; Scott A. Walper[1]; Kendrick B. Turner[1]; *[1]Center for Bio/Molecular Science & Engineering, Naval Research Laboratory, Washington, DC*

WP 593 **Middle-Down Analysis of Muropeptides Alteration in Stenotrophomonas maltophilia Cell Wall**; Yun Lin[1]; Yi-Wei Huang[2]; Chin Lin[3]; Yu Wang[2, 4]; Yi-Tsung Lin[5, 6]; Tsuey-Ching Yang[2]; Cheng-Chih Richard Hsu[1]; *[1]Department of Chemistry, National Taiwan University., Taipei, Taiwan; [2]Department of Biotechnology and Laboratory Science in Medicine, National Yang-Ming University, Taipei, Taiwan; [3]School of Public Health, National Defense Medical Center, Taipei, Taiwan; [4]Department of Laboratory Medicine, Chang Gung Memorial Hospital Linkou Branch, Taoyuan, Taiwan; [5]Division of Infectious Diseases, Department of Medicine, Taipei Veterans General Hospital, Taipei, Taiwan; [6]School of Medicine, National Yang-Ming University, Taipei, Taiwan*

WP 594 **Rapid Screening of Peptide Impurities in Calcitonin-Salmon Nasal Spray Using Data-Dependent LC-MS-MS**; Jingyue Yang[1]; Priyanka Chitranshi[1]; Ilan Geerlof-Vidavsky[1]; Kui Zeng[1]; David A. Keire[1]; Michael Trehy[1]; Wenlei Jiang[2]; Deyi Zhang[2]; Xiaohui Jiang[2]; Daniela Verthelyi[3]; *[1]Division of Pharmaceutical Analysis, Office of Testing and Research, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, St. Louis, MO; [2]Office of Research and Standards, Office of Generic Drugs, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, Silver Spring, MD; [3]Office of Biotechnology Products, Office of Pharmaceutical Quality, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, Silver Spring, MD*

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WP 595 **Selective Isolation of Tyrosine-Phosphorylated Protein by Magnetic Nanoparticles Composites**; Meng-han Liu[1]; He-Hsuan Hsiao[1]; *[1]Department of Chemistry, National Chung-Hsing University, Taichung, Taiwan*

WP 596 **Automated High-Throughput Phosphopeptides Enrichment using TiO2 Dispersive Pipette Extraction**; Sunil Hwang[1]; Todd Mulis[1]; Jingyun lee[2]; Michael Mouridian[3]; Cristina Furdui[2]; Andrew Lee[1]; *[1]Integrated Micro-Chromatography Systems, LLC, Irmo, SC; [2]Proteomics and Metabolomics Shared Resource, Wake Forest School of Medicine, Winston-Salem, NC; [3]Hamilton Robotics, Reno, NV*

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WP 598 **Robust, Sensitive, and Automated Phosphopeptide Enrichment Optimized for Low Sample Amounts Applied to Primary Hippocampal Neurons**; Harm Post[1]; Renske Penning[2]; Martin A. Fitzpatrick[2]; Luc B. Garrigues[2]; Wei Wu[2]; Harold D. MacGillavry[2]; Casper C. Hoogenraad[2]; Albert J. R. Heck[2]; A.F. Maarten Altelaar[2]; *[1], Utrecht, Utrecht; [2]Utrecht University, Utrecht, Netherlands*

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WP 611 **Why are Electron Ionization Mass Spectra of Phenyl Methyl Cyclosiloxane Polymers So Difficult to Interpret?** ; Tanya Habitz[1]; Ron Tecklenburg[1]; Amanda Palumbo[1]; *[1]Dow Corning Corporation, Auburn, MI*

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WP 617 **Identification of Novel Print-Related Contaminants in Polymeric Food Packaging**; Miguel A. Lago[1]; Luke K Ackerman[2]; *[1]University of Santiago de Compostela, Santiago de Compostela, Spain; [2]FDA/CFSAN, College Park, MD*

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WP 665 **A Targeted Mass Spectrometry Assay for Detection of HIV Gag Protein Following Induction of Latent Viral reservoirs**; Daniela M Schlatzer[1]; Aiman A. Haqqani[2]; Xiaolin Li[2]; Mark R. Chance[2]; John C. Tilton[2]; *[1]Case Western Reserve University, Cleveland , OH; [2]Center for Proteomics and Bioinformatics, Case Western Reserve University, Cleveland, OH*

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WP 670 **Time-resolved Global and Chromatin Proteomics during Herpes Simplex Virus (HSV-1) Infection**; Katarzyna Kulej[1, 2]; Daphne C. Avgousti[1, 2]; Simone Sidoli[3, 4]; Christin Herrmann[2, 5]; Ashley N. Della Fera[2]; Eui Tae Kim[1, 2]; Benjamin A. Garcia[3, 4]; Matthew D. Weitzman[1, 2]; *[1]Department of Pathology and Laboratory Medicine, University of Pennsylvania Perelman School of Medicine, Philadelphia, PA; [2]Division of Cancer Pathobiology, Children's Hospital of Philadelphia, Philadelphia, PA; [3]Department of Biochemistry and Biophysics, University of Pennsylvania Perelman School of Medicine, Philadelphia, PA; [4]Epigenetics Institute, University of Pennsylvania Perelman School of Medicine, Philadelphia, PA; [5]Cell and Molecular Biology Graduate Group, University of Pennsylvania Perelman School of Medicine, Philadelphia, PA*

WP 671 **Toward Detection of Toxoplasmosis Reactivation from Urine Using Hydro-Gel Nanoparticles and Parallel Reaction Monitoring on an Orbitrap Fusion Mass Spectrometer**; Paul Russo[1]; Hannah Steinberg[2]; Alessandra Luchini[1]; Emanuel Petricoin[1]; Lance Liotta[1]; Robert H. Gilman[2]; Toxoplasmosis Working Group Universidad Peruana Cayetano Heredia[3]; *[1]George Mason University, Manassas, VA; [2]Johns Hopkins University, Baltimore, MD; [3]Toxoplasmosis Working Group at Universidad Peruana Cayetano Heredia, Lima, Peru*

WP 672 **The DNA Sensor IFIX Suppresses Viral Gene Transcription during HSV-1 Infection and is Counteracted by Virus-Induced Proteasomal Degradation**; Marni Crow[1]; Ileana Cristea[1]; *[1]Princeton University, Princeton, NJ*

WP 673 **Deciphering Human Sirtuin 3 Antiviral Functions and its Dynamic Regulation of the Mitochondria Acetylome during Infection**; Xinlei Sheng; *Princeton University, Princeton, NJ*

WP 674 **A Chemical Proteomic Strategy to unravel the Infectious Zika Virus Entry into Host Cells**; Mayank Srivastava[1]; Andrew Miller[1]; Yuan Zhou[1]; Richard Kuhn[1]; Andy Tao[1]; *[1]Purdue University, West Lafayette*

WP 675 **Putative Antimicrobial Peptides in the Lobster, Homarus americanus: Identification Using Top-Down and Bottom-Up Proteomics Coupled with Transcriptomics**; Daniel Do[1]; Giap H. Vu[1]; Patsy S. Dickinson[1]; Andrew E. Christie[2]; Elizabeth A. Stemmler[1]; *[1]Bowdoin College, Brunswick , ME; [2]University of Hawaii at Manoa, Honolulu, Hawaii*

WP 676 **Divergent and Coordinated Immune-Regulatory Roles of the Viral DNA Sensors IFI16 and cGAS during Viral Infection**; Krystal K Lum[1]; Benjamin A Diner[1]; Bokai Song[1]; Ileana M Cristea[1]; *[1]Princeton Universitry, Princeton, NJ*

PROTEOMICS: INTACT PROTEINS
677 - 686

WP 677 **Nucleotide Ligand Binding and Exchange in Recombinant KRAS Using Native Mass Spectrometry**; Hemanth Akkiraju[1]; Anna Kaplan[1]; Lewis M. Brown[1]; Brent R. Stockwell[1]; *[1]Columbia University, New York , NY*

WP 678 **Separation and Identification of Mouse Brain Microproteins using Top-down Method with High Resolution Nanocapillary Liquid Chromatography Mass Spectrometry**; Wenxue Li[1]; Filomena Petruzziello[1]; Nan

Zhao[2]; Huiyuan Zhao[2]; Xueting Ye[2]; Xiaozhe Zhang[2]; Gregor Rainer[1]; *[1]University of Fribourg, Fribourg, Switzerland; [2]Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China*

WP 679 **Quantification of Proteoforms and Construction of Proteoform Families**; Michael R. Shortreed[1]; Anthony J. Cesnik[2]; Brian L. Frey[2]; Leah V. Schaffer[2]; Rachel A. Knoener[2]; Mark Scalf[2]; Lloyd M. Smith[2]; *[1]University of Wisconsin, Madison, WI; [2]University of Wisconsin, Madison, WI*

WP 680 **Method Development for Comprehensive Two Dimensional Liquid Chromatographic Separation and Triple Quadrupole Mass Spectrometric Quantitation of Intact Proteins**; Dananjaya Kalu Appulage[1]; Yehia Z Baghdady[1]; Evelyn H Wang[2]; Jorge Smith[2]; Ty Kahler[3]; Kevin A. Schug[1]; *[1]University of Texas at Arlington, Arlington, TX; [2]Shimadzu Scientific Instruments, Columbia, MD; [3]Restek Corporation, Bellefonte, PA*

WP 681 **High Sensitivity and Accurate Mass Analyses of Intact Human Endogenous Proteins Produced Innaïve CD4 Cells using Nano Flow LC-MS**; Jason X. Tang[1]; Kyoung-soo Choi[1]; Stuart Bright[1]; Chetan Patel[1]; *[1]Eli Lilly & Company, Branchburg, NJ*

WP 682 **Elucidating E. coli Proteoform Families Using a Global PTM Discovery Database and Intact-mass Proteomics**; Yunxiang Dai[1]; Robert J. Millikin[1]; Anthony J. Cesnik[1]; Michael R. Shortreed[1]; Mark Scalf[1]; Brian L. Frey[1]; Lloyd M. Smith[1]; *[1]University of Wisconsin-Madison, Madison, WI*

WP 683 **Using Random Sampling Statistics to Model Protein Isotope Distributions**; Zachary Philip Gotlib[1]; Peter T. A. Reilly[2]; *[1]Washington State University, Pullman, WA; [2]Washington State University, Pullman, WA*

WP 684 **Evidence for Glycation/Glycosylation of Low Molecular Weight Gluten Polymer Subunits in Wheat Kernels**; Ray Bacala[1, 2]; Hélène Perreault[2]; Dave Hatcher[1]; *[1]Canadian Grain Commission, Winnipeg, MB; [2]Department of Chemistry, University of Manitoba, Winnipeg, MB*

WP 685 **High Resolution LC-ESI-MS of Intact Wheat High Molecular Weight Glutenin Subunits (HMWGS) Reveals Unexpected Heterogeneity**; Katherine Cordova[1]; Ray Bacala[1]; Dave Hatcher[1]; *[1]Canadian Grain Commission, Winnipeg, MB*

WP 686 **Dynamic pH Junction Based Capillary Zone Electrophoresis-Mass Spectrometry with Half-a-Microliter Loading Capacity for Top-Down Intact Protein Characterization**; Eli McCool[1]; Rachele Lubeckyj[1]; Liangliang Sun[1]; *[1]Department of Chemistry, Michigan State University, East Lansing, MI*

PROTEOMICS: QUANTITATIVE III
687 - 706

WP 687 **Whole and Phosphoproteome Analysis of Epithelial to Mesenchymal Transition in ES Derived RPE**; Joseph Leo Mertz[1]; Srinivas R Sripathi[1]; Xue Yang[1]; David Clark[1]; Lijun Chen[1]; Noriko Esumi[1]; Hui Zhang[1]; Donald J Zack[1]; *[1]Johns Hopkins University School of Medicine, Baltimore, MD*

WP 688 **Systematic Proteome Profiling by DIA-MS to Characterize Calorie Restriction-Induced Life Span Extension in Yeast**; Lindsay K Pino[1]; Matt Kaeberlein[1]; Andrew N. Hoofnagle[1]; William S Noble[1]; Michael J MacCoss[1]; *[1]University of Washington, Department of Chemistry, Seattle, WA*

WP 689 **Quantitative Temporal Proteomics Analysis of Murine Bone Marrow Macrophages and RAW264.7 Cells in Osteoclast Differentiation**; Andrew Ng[1]; Chengjian Tu[2, 3]; Shichen Shen[3, 4]; Jun Li[2, 3]; Jun Qu[2, 3, 4]; Shuying Yang[5]; *[1]Department of Oral Biology, School of Dental Medicine, University at Buffalo, State University of New York, Buffalo, NY; [2]Department of Pharmaceutical Sciences, University at Buffalo, State University of New York, Buffalo, NY; [3]New York State Center of Excellence in Bioinformatics and Life Sciences, Buffalo, NY; [4]Department of Biochemistry, School of Medicine and Biomedical Sciences, University at Buffalo, State University of New York, Buffalo, NY; [5]Department of Anatomy and Cell Biology, School of Dental Medicine, University of Pennsylvania, Philadelpha, PA*

WP 690 **Quantitative Proteomics Analysis of Heat Shock Proteins Involved in Unfolded Protein Response in Glioblastoma Cell Lines Induced by Different Drugs**; Jose Cesar Rosa[1]; Helen Julie Laure[1]; Carolina Thome[1]; Germano Ferreira[1]; Suely K.N. Marie[2]; Sueli Oba Shinjo[2]; Clarice Izumi[1]; *[1]Medical School of Ribeirao Preto University of Sao Paulo, Ribeirao Preto, SP; [2]Medical School of Sao Paulo University of Sao Paulo, Sao Paulo, Brazil*

WP 691 **Quantitative Profiling of Snake Venom using TMT Protein Labeling and Top-Down Mass Spectrometry**; Dahang Yu[1]; Zhe Wang[1]; Hongyan Ma[1]; Si Wu[1]; *[1]University of Oklahoma, Norman, OK*

WP 692 **Quantification of Metabolic Enzymes in the IDH1/2 Metabolic Pathways of Glioma Tissue using PRM**; Lennard J.M. Dekker[1]; Suying Wu[1]; Johan M. Kros[1]; Dana Mustafa[1]; Theo M. Luider[1]; *[1]Erasmus Medical Center, Rotterdam, Zuid Holland*

WP 693 **Temporal Transcriptomic and Proteomic Landscapes of Pancreatic Islets in Type 2 Diabetic Rats**; Junjie Hou[1]; Zonghong Li[2]; Wen Zhong[3]; Qiang Hao[1]; Dongyu Zhao[1]; Lei Lei[1]; Linlin Wang[1]; Pingyong Xu[1]; Yifa Zhou[2]; You Wang[1]; Tao Xu[1]; *[1]Institute of Biophysics, CAS, Beijing, China; [2]Northeast Normal University, Changchun, China; [3]HuaZhong University of Science and Technology, Wuhan, China*

WP 694 **Enhanced Analysis of Host Cell Proteins from CHO cell cultured mAb using LC/MS**; Linfeng Wu[1]; Jordy J. Hsiao[1]; Te-Wei Chu[1]; Pat Perkins[1]; *[1]Agilent Technologies, Santa Clara, CA*

WP 695 **Targeted Quantification of Protein Phosphorylation in the Epidermal Growth Factor Receptor Signaling Pathway**; Lian Yi[1]; Tujin Shi[2]; Fillmore L Thomas[2]; Marina A Gritsenko[2]; Yuqian Gao[2]; Tao Liu[2]; Richard D Smith[2]; Steven H Wiley[2]; Wei-Jun Qian[2]; *[1], Richland, WA; [2]PNNL, Richland, WA*

WP 696 **Organ-Level Proteomics of Systemic Infection Illuminates Dynamic Responses in a Mouse Model**; John Lapek[1]; Robert Mills[1]; Ronnie Fang[1]; Brian Luk[1]; Liangfang Zhang[1]; Rob Knight[1]; David Gonzalez[1]; *[1]UCSD, La Jolla, CA*

WP 697 **Quantitative Proteomic Approach Reveals Landscape of the Regulatory Elements for Lysineβ-hydroxybutyrylation Pathway**; He Huang[1]; Di Zhang[1]; Yingming Zhao[1]; *[1]University of Chicago, Chicago, IL*

WP 698 **Quantitative Multi-omics Characterization of Gemcitabine-induced Apoptosis and Resistance in Human Pancreatic Cancer Cells**; Xiaofang Zhong[1]; Ling Hao[1]; Jillian Johnson[1]; Dustin Frost[1]; Amanda Buchberger[1]; John Kao[2]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI; [2]Hong Kong University of Science and Technology, Hong Kong, China*

WP 699 **Characterizing Signaling Networks Associated with AMPK Activation in Human Myotubes by Isobaric Chemical Labeling Quantitative Phosphoproteomics**; Chuong Nguyen[1]; Maryann Whitley[2]; Russell Miller[2]; Kimberly Cameron[2]; Ravi Kurumbail[3]; Kieran Geoghegan[3]; *[1]Pfizer, Groton, CT; [2]Pfizer, Cambridge, MA; [3]Pfizer, Groton, CT*

WP 700 **Quantitative Proteomic Analysis of Glucose Fasting Prior to Tandem Anti-Autophagy and Chemotherapy Treatment in Colorectal Cancer**; Monica Schroll[1]; Gabriel LaBonia[1]; Amanda B. Hummon[1]; *[1]University of Notre Dame, Notre Dame, IN*

WP 701 **3D Imaging and Quantitative Proteomic Characterization of Bladder Stones and their Matrix Investigating a Cystinuria Mouse Model**; Tiffany Zee[1];

Sruthi Damodar[1]; Bradford W Gibson[1, 2]; Marshall Stoller[3]; Pankaj Kapahi[1]; Birgit Schilling[1]; *[1]Buck Institute for Research on Aging, Novato, CA; [2]Amgen, South San Francisco, CA; [3]University of California, San Francisco, San Francisco, CA*

WP 702 **Functional Consequences of Mutations in the Mammalian Target of Rapamycin Signaling Cascade**; Cassandra Wong[1, 2]; Geoffrey Hesketh[1]; Anne-Claude Gingras[1, 2]; *[1]Lunenfeld-Tanenbaum Research Institute, Toronto, ON, Canada; [2]Department of Molecular Genetics, University of Toronto, Toronto, ON, Canada*

WP 703 **Quantitative Proteomics in a Non-Sequenced Vole Model: Insights into the Role of Brown Adipose Tissue Against Obesity**; Margaux Benhaim-Delarbre[1]; Barbara Henning[2]; Georg Tascher[1]; Pierre Bize[3]; Fabrice Bertile[1]; *[1]Institut Pluridisciplinaire Hubert Curien, CNRS, LSMBO,Université de Strasbourg, Strasbourg, France; [2]Brazilian Institute of Neuroscience and Neurotechnology (BRAINN), University of Campinas, Brazil, Campinas, Brazil; [3]Institute of Biological and Environmental Sciences, University of Aberdeen, Aberdeen, UK*

WP 704 **Gender-Specific Protein Expression of Lymphoblasts using Label Free LC/MS/MS**; Kathleen C Lundberg[1]; Nicholas Szoko[2]; Daniela M Schlatzer[3]; Marvin R Natowicz[2]; *[1]Case Western Reserve University, Cleveland, OH; [2]Cleveland Clinic Foundation, Cleveland, Ohio; [3]Case Western Reserve University, Cleveland , OH*

WP 705 **Proteomic Storage Study of Priobiotics**; Barbara S. Larsen[1]; Ron Agee[2]; Michael Dauner[3]; Kurt Fenster[2]; Chris Hollard[2]; Cathy Kalbach[3]; Sunny Li[3]; Buffy Stahl[2]; Tom Mower[3]; Alexander Kopatsis[3]; Corban Rivera[3]; *[1]The DuPont Company, Wilmington, DE; [2]DuPont, Madison, Wi; [3]DuPont, Wilmington, DE*

WP 706 **A Mass Spectrometry-Based Proteomic Method to Discover RNA Binding Protein Complexes in Developing Rice Seeds**; Youngwoo Lee[1]; Zach McBride[1]; Daniel Szymanski[1]; *[1]Purdue University, West lafayette, IN*

SYSTEMS BIOLOGY II
707 - 719

WP 707 **An Unbiased Protein Association Study on the Public Human Proteome Reveals Biological Connections between Co-Occurring Protein Pairs**; Surya Gupta[1, 2, 3]; Kenneth Verheggen[1, 2, 3]; Jan Tavernier[1, 3]; Lennart Martens[1, 2, 3]; *[1]Department of Biochemistry, Ghent University, Ghent, Belgium; [2]Bioinformatics Institute Ghent, Ghent University, Ghent, Belgium; [3]Vib-Ugent Center For Medical Biotechnology, Ghent, Belgium*

WP 708 **Proteomic Analysis Reveals Novel Hydroxyproline-Dependent Cellular Pathways in Cancer Cells**; Luke Erber[1]; Tong Zhou[2]; Yue Chen[2]; *[1]University of Minnesota, Minneapolis, MN; [2]University of Minnesota, Minneapolis, MN*

WP 709 **High pH Fractionation for Enhancing the Proteome Coverage in Tissues Dissected from the Early Frog (Xenopus laevis) Embryo**; Aparna B. Baxi[1, 2]; Camille Lombard-Banek[1]; Sally A. Moody[2]; Peter Nemes[1]; *[1]Department of Chemistry, The George Washington University, Washington, D.C.; [2]Department of Anatomy & Regenerative Biology, The George Washington University, Washington, D.C.*

WP 710 **Multi-Omics Comparative Analysis Reveals Host Signaling Pathways Affected by the Gut Microbiota**; Nathan P Manes[1]; Natalia Shulzhenko[2]; Arthur G Nuccio[1]; Sara Azeem[1]; Andrey Morgun[2]; Aleksandra Nita-Lazar[1]; *[1]National Institutes of Health, Bethesda, MD; [2]Oregon State University, Corvallis, OR*

WP 711 **A Multiproteomic Approach to Characterize Transcriptional Regulators of HIV Expression During Activation of Primary CD4+T Cell Hosts**; Mei Leng[1]; Alexander Saltzman[1]; Bhoomi Bhatt[1]; Anna Malovannaya[1]; *[1]Baylor College of Medicine, Houston, TX*

WP 712 **In-depth Analyses of Protein Abundance, Phosphorylation, Synthesis and Degradation during Neuronal Development and Synaptic Plasticity**; Renske Penning[1]; Christian K. Frese[1]; Charlotte A.G.H. van Gelder[1]; Marina Mikhaylova[1]; Riccardo Stucchi[1]; Harm Post[1]; Albert J. R. Heck[1]; Harold D. MacGillavry[1]; Casper C. Hoogenraad[1]; A.F. Maarten Altelaar[2]; *[1]Utrecht University, Utrecht, Netherlands; [2] Utrecht University, Utrecht*

WP 713 **Quantitative Proteomics and Immunohistochemistry Reveal Insights into Cellular and Molecular Processes in the Infarct Border Zone after Myocardial Infarction**; Zachery R Gregorich[1]; Libang Yang[2]; Wenxuan Cai[3]; Patrick Zhang[2]; Bernice Young[2]; Yiwen Gu[3]; Jianyi Zhang[4]; Ying Ge[3]; *[1]UW Madison, Madison, WI; [2]University of Minnesota, Minneapolis, MN; [3]University of Wisconsin Madison, Madison, WI; [4]University of Alabama at Birmingham, Birmingham, AL*

WP 714 **Pathway Visualization and Analysis for Quantitative Posttranslational Modification and Proteome Time Series Data in the Perseus Software**; Jan Rudolph[1]; Stefka Tyanova[2]; John C. Rogers[3]; Bhavin Patel[3]; Shouling Xu[4, 5]; Devin Drew[5]; Kai Fritzemeier[6]; Andreas F. Huhmer[7]; Juergen Cox[1]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany; [2]Hoffmann-La Roche, Basel, Switzerland; [3]Thermo Fisher Scientific, Rockford, IL; [4]Stanford University School of Medicine, Palo Alto, CA; [5]Thermo Fisher Scientific, San Jose, CA; [6]Thermo Fisher Scientific, Bremen, Germany; [7]Thermo Fisher, San Jose, CA*

WP 715 **Analysis of Neonatal Mouse Hearts with Shotgun Proteomics and Untargeted Metabolomics**; Päivi Pöhö[1]; Jaakko Teppo[1, 2]; Virpi Talman[3]; Anu Vaikkinen[1]; Sini Kinnunen[3]; Kajetan Trost[4]; Tommi Suvitaival[4]; Peter Rossing[4]; Tapio Kotiaho[1, 5]; Heikki Ruskoaho[3]; Markku Varjosalo[2]; Risto Kostiainen[1]; *[1]Division of Pharmaceutical Chemistry and Technology, Faculty of Pharmacy, University of Helsinki, Helsinki, Finland; [2]Molecular Systems Biology Research Group and Proteomics Unit, Institute of Biotechnology, University of Helsinki, Helsinki, Finland; [3]Division of Pharmacology and Pharmacotherapy, Faculty of Pharmacy, University of Helsinki, Helsinki, Finland; [4]Steno Diabetes Center Copenhagen, Gentofte, Denmark; [5]Department of Chemistry, Faculty of Science, University of Helsinki, Helsinki, Finland*

WP 716 **Broad-scale Proteomic Analysis of Subcellular Fractions for the High-Throughput Investigation of Mechanism of Action**; Danielle B. Gutierrez[1]; Melissa A. Farrow[2]; Carrie E. Romer[1]; Jamie L. Allen[1]; Yuan-wei Nei[1]; Jocelyn Simpson[2]; Tina Tsui[1]; Salisha Hill[1]; Kristie L. Rose[1]; Jeremy L. Norris[1]; D. Borden Lacy[2]; Eric P. Skaar[2]; Richard M. Caprioli[1]; *[1]Vanderbilt University, Nashville, TN; [2]Vanderbilt University Medical Center, Nashville, TN*

WP 717 **Quantitative Multidimensional Characterization of Protein-Protein Interactions in Cancer**; Danielle Swaney[1]; Margaret Soucheray[1]; Nevan Krogan[1]; *[1]UCSF, San Francisco, CA*

WP 718 **REPRINT:** A **R**esource for **E**valuation of **Pr**otein **Int**eraction Networks; Dattatreya Mellacheruvu[1]; Zachary Wright[1]; Felipe da Veiga Leprevost[1]; Anne-Claude Gingras[2]; Alexey I. Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI; [2]Lunenfeld-Tanenbaum Research Institute, Toronto, ON, Canada*

WP 719 **Mapping Ubiquitin Regulation under Stress by Multi-Dimensional Proteomics**; Jeremy O'Connell[1]; Marta Isasa[2]; Joao Paulo[1]; Steven Gygi[1]; *[1]Harvard Medical School, Boston, MA; [2]C4 Therapeutics, Cambridge, MAPharma Services, Inc., Lincolnshire, IL; [4]Q² Lab Solutions Bioanalytical and ADME Labs, Ithaca, NY; [5]Quintiles, Ithaca, NY*

BIOMARKERS: DISCOVERY II
001 - 024

ThP 001 **Biomarker Discovery in Fragile X-Associated Tremor/ Ataxia Syndrome Using Mass Spectrometry Based Proteomics**; Amber Orcutt[1]; Vadi Bhat[2]; Carol Haney-Ball[2]; Deborah A. Hall[1]; Stephanie Cologna[3]; Elizabeth M. Berry-Kravis[1]; *[1]Rush University, Chicago, IL; [2]Agilent Technologies, Wilmington, DE; [3]University of Illinois at Chicago, Chicago, Illinois*

ThP 002 **Annexin A10 is a Candidate Marker Associated with the Progression of Pancreatic Precursor Lesions to Adenocarcinoma**; Jianhui Zhu[1]; Jing Wu[1]; Xiucong Pei[1]; Zhijing Tan[1]; Mingrui An[1]; Jiaqi Shi[1]; David M. Lubman[1]; *[1]University of Michigan Medical Center, Ann Arbor, MI*

ThP 003 **Cross-Panel Analysis of INLIGHT™ N-Linked Glycans in the Avian Model of Ovarian Cancer**; Elizabeth S. Hecht[1]; Alison A. Motsinger-Reif[1]; David C. Muddiman[1]; *[1]North Carolina State University, Raleigh, NC*

ThP 004 **Development of a Novel Chemical Method for Serum/ Plasma Protein Depletion**; Anton Iliuk[1]; Li Li[1]; Keerthi Jayasundera[2]; Andy Tao[1, 2]; *[1]Tymora Analytical Operations, West Lafayette, IN; [2]Purdue University, West Lafayette, IN*

ThP 005 **Discovery of Exposure Markers of di(2-pro,pylheptyl) phthalate (DPHP) Using Mass Spectrometry and Two Data Screening Procedures**; Pao-Chi Liao[1]; Chia-Lung Shih[1]; Pao-Mei Liao[2]; Jen-Yi Hsu[1]; *[1]Department of Environmental and Occupational Health, College of Medicine, National Cheng Kung University, Tainan, Taiwan; [2]Department of Environmental Science and Property Management, Jinwen University of Science and Technology, New Taipei City, Taiwan*

ThP 006 **Identification of Hypoxia-Induced Splicing Variants in Cancer Cells Using Proteomics Approach**; Pang-Hung Hsu[1]; Chia-Hung Li[1]; *[1]National Taiwan Ocean University, Keelung, Taiwan*

ThP 007 **Morphology Mass Spectrometry Imaging to Discover Heterogeneity Markers in Oncology**; Gael Picard de Muller[1]; Rima Ait-Belkacem[1]; Fabien Pamelard[1]; David Bonnel[1]; Jonathan Stauber[1]; *[1]Imabiotech, Loos, France*

ThP 008 **Identification of Cerebrospinal Fluid Peptide Markers for Recurrent Malignant Brain Tumor by Quantitative Proteomics**; Tomohiro Kohata; *Shingo Ito, Kumamoto, Japan; Mio Hirayama, Kumamoto, Japan; Takuya Furuta, Kanazawa, Japan; Mitsutoshi Nakada, Kanazawa, Japan; Sumio Ohtsuki, Kumamoto, Japan*

ThP 009 **Screening of Diabetes Mellitus, Colorectal Cancer Complicated with Diabetes and Colorectal Cancer by Simultaneous Targeted and Non-Targeted Quantitative Metabolomics Analysis**; Yang Gao; *Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing, China*

ThP 010 **Parkinson's Disease Cerebral Spinal Fluid Analysis by Direct Injection Electrosonic Spray Ionization Multiple Reaction Monitoring-Profiling**; Karen E. Yannell[1]; Christina R. Ferreira[2]; Tiago JP Sobreira[2]; R. Graham Cooks[2]; *[1]Purdue University, west lafayette, IN - Indiana; [2]Purdue University, West lafayette, Indiana*

ThP 011 **Comprehensive, Unbiased Proteomic Profilingof the Cell-Surface, Exosomal, and Secreted Proteomes of Senescent Cells**; Natan Basisty[1]; Bradford W Gibson[1]; Judith Campisi[1]; Birgit Schilling[1]; *[1]The Buck Institute for Research on Aging, Novato, CA*

ThP 012 **Quantification of *in vivo* Protein Molecular Dynamics Employing Stable Isotope Labeling with Deuterium Oxide and High Resolution Mass Spectrometry**; Thomas E Angel[1]; Matthew E Szapacs[1]; Zhuo Chen[1]; Christopher A Evans[1]; *[1]GSK, King of Prussia, PA*

ThP 013 **Proteomic Analyses of GNMT Knock-Out Mice – the Translational Research Study of mARC Genes Related to Liver Cancer**; Ming-Hui Yang[1]; Yi-Ming Arthur Chen[1]; Hsiao-Hsuan Mo[1]; Yu-Chang Tyan[1]; *[1]Kaohsiung Medical University, Kaohsiung, Taiwan*

ThP 014 **Identification and Label-Free Quantification of Lipid Based Markers for Pre-Term Birth Using a Novel Scanning Quadrupole DIA Acquisition Method**; Lee A Gethings[1]; Shirish Yakkundi[2]; Gregoire Thomas[3]; Aude-Clare Morillon[2]; James I Langridge[1]; Louise Kenny[2]; *[1]Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK; [2]INFANT, Cork, Ireland; [3]Squ4re, Wevelgem, Belgium*

ThP 015 **Determination of Metabolomics Profile Changes for Prediction of Mortality in Induced Hypothermia after Cardiac Arrest Patients**; Urszula Osinska Warncke[1]; Mary Ann Peberdy[1]; Dayanjan S Wijeisnghe[1]; *[1]Virginia Commonwealth University, Richmond, Virginia*

ThP 016 **Deepest Plasma Proteome Coverage with Lumos**; Yue Zhou[1]; Aiying Nie[2]; Jing Li[1]; *[1]ThermoFisher Scientific, Shanghai, China; [2]ThermoFisher Scientific, shanghai, China*

ThP 017 **Discovery and Characterization of Leukemia Chemotherapy-Related Neurotoxicity Biomarkers in Cerebrospinal Fluid via Mass Spectrometry-based Shotgun Proteomics**; Qinying Yu[1]; Bingming Chen[1]; Yu Feng[1]; Chrysanthy Ikonomidou[1]; Lingjun Li[1]; *[1]University of Wisconsin Madison, Madison, WI*

ThP 018 **Probing Exosomes for Early-Stage Biomarkers of Coronary Artery Disease**; Sarah Elder[1]; Blair Chen[1]; Weiguo Andy Tao[1]; *[1]Purdue, West Lafayette, IN*

ThP 019 **Optimizing Differential Ion Mobility-Mass Spectrometry based Leukemia Antigen Detection**; Ian M Schlup[1]; James E Keating[1]; Sally Hunsucker[2]; Courtney Elliot[2]; Paul Armistead[2]; Gary L Glish[1]; *[1]University of North Carolina at Chapel Hill, Department of Chemistry, Chapel Hill, NC; [2]Lineberger Comprehensive Cancer Center, Chapel Hill, NC*

ThP 020 **Identification, Validation and Quantification of Neuregulin-4 by Immunoreactive Methods in Blood Samples from Patients With or Without Diabetes**; Rong-Ming Lyu[1]; Nae J Dun[2]; Xianghai Yao[1]; Qing Tian[1]; Siok Le Dun[2]; Jin Jun Luo[2]; Jaw-Kang Chang[1]; *[1]Phoenix Pharmaceuticals, Burlingame, CA; [2]Temple University, Philadelphia, PA 19140*

ThP 021 **Analysis of Cellular and Exosomal Proteins to Decode LKB1 Regulated Pathways in Lung Cancer Invasion and Metastasis**; Bernice Agana[1]; Michael Koenig[2]; Takehito Shukuya[2]; Joseph Amann[2]; David Carbone[2]; Vicki Wysocki[1]; *[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; [2]Department of Internal Medicine, The Ohio State University, Columbus, OH*

ThP 022 **MIK-MS (Molecular Interaction and Kinetics Mass Spectrometry) Used to Verify the Affinity Ranking of Protein-Small Molecule Interactions**; Tetsuya Fukuda[1]; Naoko Obi[2]; Noboru Nakayama[3]; John Ervin[4]; Yasuhiko Bando[1]; Toshihide Nishimura[3]; Toshiaki Somehara[2]; Satoru Nagatoishi[5]; Kouhei Tsumoto[6]; Takeshi Kawamura[7]; *[1]Research and Development, Biosys Technologies, Inc., Meguro-ku, Japan; [2]Research & Marketing, Nissha Printing Co., Ltd., Kyoto-shi, Japan; [3]Translational Medicine Informatics, St. Marianna University School of Medicine, Kawasaki-shi, Japan; [4]Silicon Kinetics, Inc., San Diego, CA; [5]School of Engineering, The University of Tokyo, Minato-ku, Japan; [6]School of Engineering, The Institute of Medical Science, and Drug Discovery Initiative, The University of Tokyo, Minato-ku, Japan; [7]Proteomics Laboratory, Radioisotope Center, The University of Tokyo, Bunkyo-ku, Japan*

ThP 023 **Methods in Purity Optimization for A1AT Glycopeptide Analysis in Biomarker Research**; Elisa Warner[1]; Jianhui Zhu[2]; David M. Lubman[2]; *[1], Ann Arbor, MI; [2]University of Michigan Medical School, Ann Arbor, MI*

ThP 024 **Identification of Single Amino Acid Variants from Three Subpopulations in the MCF-7 Breast Cancer Cell Line**; Zhijing Tan[1]; Song Nie[1, 2]; Sean P. McDermott[1]; Max S. Wicha[1]; David M. Lubman[1]; *[1]The University of Michigan, Ann Arbor, MI; [2]Pacific Northwest National Laboratory, Richland, WA*

BIOMARKERS: QUANTITATIVE ANALYSIS III
025 - 051

ThP 025 **Using SRM to Monitor Biomarkers for Clostridium Difficile Susceptibility.**; Sigmund J Haidacher[1, 2]; Kathleen M Hoch[1, 2]; Prapaporn Boonma[2, 3]; Jennifer M Auchtung[3]; Robert A Britton[3]; Tor Savidge[2, 3]; Anthony M Haag[2, 3]; *[1]Baylor College of Medicine, Houston, TX; [2]Texas Children's Hospital, Houston, TX; [3]Baylor College of Medicine, Houston, TX*

ThP 026 **Function of Human Gut Microbiome in Chronic Kidney Disease: Metaproteomics Approach**; Oleg K Karaduta[1]; Gerren P Hobby[1]; Galina V Glazko[1]; Yasir Rahmatallah[1]; Lisa M Orr[1]; Samuel G Mackintosh[1]; Ricky D Edmondson[1]; John M Arthur[1]; Boris L Zybaylov[1]; *[1]UAMS, Little Rock, AR*

ThP 027 **Pre-Analytical Variability Assessment for Human Plasma Samples Based on Inflammation Biomarkers and Abundant Proteins**; Zhijun Cao[1]; Jinchun Sun[1]; Laura Schnackenberg[1]; Lisa Pence[1]; Tom Schmitt[1]; Mackean Maisha[1]; Antje Wagner-Golbs[2]; Beate Kamlage[2]; Richard D Beger[3]; Li-Rong Yu[1]; *[1]National Center for Toxicological Research, FDA, Jefferson, AR; [2]Metanomics GmbH, Berlin, Germany; [3]NCTR/FDA, Jefferson, AR*

ThP 028 **Don't Know Activity from ADAM(TS13)? The First LC-MS/MS Assay for Measuring Activity of von Willebrand Factor Cleaving Protease**; Meghan Bradley[1]; Russell Grant[1]; Christopher M Shuford[1]; *[1]LabCorp, Burlington, NC*

ThP 029 **Quantification of Bile Acids and their Conjugates in Plasma by Liquid Chromatography/Full Scan High Resolution Mass Spectrometry**; Yao Shi[1]; Michael Van Parys[1]; Yang Gao[1]; Dennis Milanowski[1]; Stephanie Cape[1]; Xiaorong Liang[2]; Brian Dean[2]; *[1]Covance, Madison, WI 53704; [2]Genentech, Inc, South San Francisco, CA*

ThP 030 **Sensitive and Reproducible LC-MS Quantification of C-Reactive Protein in Plasma Using a Generic Kit-Based Approach for Clinical Research**; Paula Orens[1]; Mary E Lame[2]; Steven Calciano[2]; Erin Chambers[2]; *[1]Waters Corporation, Milford, MA; [2]Waters Corp, Milford, MA*

ThP 031 **Glycoproteomics of Breast Cancer Human Plasma Extracellular Vesicles for Biomarker Discovery and Validation Using Polymer-Based Reverse Phase Glycoprotein Array**; Hillary Andaluz[1]; I-Hsuan Chen[1]; Li Pan[1]; Anton Iliuk[1, 2]; Andy Tao[1, 2]; *[1]Purdue University, West lafayette, Indiana; [2]Tymora Analytical Operations, West Lafayette, IN*

ThP 032 **LC/MS Analysis of Various Compounds Having Amino or Ammonium Groups with Using a New Polymer-based HILIC Column**; Junji Sasuga[1]; Daisuke Maruyama[1]; Ron Benson[2]; Leah Block[2]; *[1]Showa Denko KK, Ogimachi, Japan; [2]Shodex, Showa Denko America, Inc., New York, NY*

ThP 033 **A Simple Dilute-and-Shoot FI-MS/MS for Quantification of Glycocholic Acid in Human Bile Using Standard Addition Method**; Raghavi Kakarla[1]; Ramakrishna Reddy Voggu[1]; Baochuan Guo[2]; Janet Donaldson[3]; *[1]Cleveland State University, Cleveland, OH; [2]Cleveland State University, Department of Chemistry, Cleveland, OH; [3]Mississippi State University, Starkville, MS*

ThP 034 **Quantitative MALDI-TOF Measurements of Protein Functional Activity in Bronchoalveolar Lavage and Serum for Rapid Adverse Drug Reactions Assessment**; Ilya Toropygin[1]; Alexandr Protasov[2]; Olga Mirgorodskaya[2]; Andry Vasin[2]; Andrey Lisitsa[1]; *[1]Inst.of Biomedical Chemistry, Moscow, Moscow; [2]Research Institute of Influenza, Saint-Petersburg, Russia*

ThP 035 **Quantitation of a Broad Range of Nucleotides in Mouse Tissues Using a Novel Liquid Chromatography/Mass Spectrometry Method**; Chris Petucci[1, 2]; Andrew Zelenin[2, 3]; Nidhi Kapoor[2, 3]; Meghan Gabriel[2, 3]; Mauro Dispagna[2, 3]; Stephen J. Gardell[2, 3]; *[1]Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL; [2]University of Florida, Gainesville, FL; [3]Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL*

ThP 036 **Detection and Quantification of Bufadienolides in Complex Sample Mixtures Using a nano-ESI-IM-MS Coupled to nano-UPLC**; Luke T. Richardson[1]; Brooke A. Brown[1]; Elyssia S Gallagher[1]; Jules B. Puschett[2]; Touradj Solouki[1]; *[1]Baylor University, Waco, Texas; [2]Texas A&M University, College Station, Texas*

ThP 037 **Urinary Metabolomics and Proteomics Analysis of an E.coli-Induced Prostatic Inflammation Mouse Model via Isobaric DiLeu Tagging and Label-free Methods**; Pingli Wei[1]; Ling Hao[2]; Fengfei Ma[3]; Qing Yu[3]; Amanda Buchberger[4]; Sanghee Lee[5]; Wade Bushman[5]; Lingjun Li[1, 3]; *[1]Department of chemistry, University of Wisconsin Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [3]School of pharmacy, University of Wisconsin Madison, Madison, WI; [4]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [5]Department of Urology, University of Wisconsin-Madison, Madison, WI*

ThP 038 **Imputation of Missing Data in Quantitative Proteomics using Singular Value Thresholding**; Tjeerd Dijkstra[1]; Timo Sachsenberg[2]; Oliver Kohlbacher[3]; *[1]Max Planck Institute for*

Developmental Biology, Tuebingen, Germany; [2]Universität Tübingen, Tübingen, Germany; [3]Max Planck Institute for Developmental Biology, Tübingen, Germany

ThP 039 **Ultra-Trace Level Quantitation of Modified Human Lung DNA: Extreme Efforts to Optimize the Sensitivity of HRAM Detection of Adducted Nucleosides**; J. Bradley Hochalter[1]; Peter W. Villalta[1]; Stephen S. Hecht[1]; *[1]Masonic Cancer Center, University of Minnesota, Minneapolis, MN*

ThP 040 **Selective Enrichment of Biomarkers Using Amphiphilic Polymers for Enhanced Mass Spectrometric Analysis**; Mahalia A. C. Serrano[1]; Bo Zhao[1]; Sankaran Thayumanavan[1]; Richard W Vachet[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

ThP 041 **Protein Biomarker Discovery for Patient with Gastric Cancer Using Mass Spectrometry-Based Quantitative Urinary Proteomics**; Hong Wang[1]; Hiroaki Katayama[1]; Xiaoqian Liu[1]; Juan Chen[1]; Ayumu Taguchi[1]; Samir Hanash[1]; *[1]MD Anderson Cancer Center, Houston, TX*

ThP 042 **The Experimental Autoimmune Myocarditis in Rat Activates the Autophagy and Apoptosis**; Jong Bok Seo[1]; Seung-Min choi[1]; *[1]Korea Basic Science Institute, Seoul, Asia*

ThP 043 **A Quantitative Analytical Method for PIVKA-II Using Multiple Reaction Monitoring-Mass Spectrometry for Early Diagnosis of Hepatocellular Carcinoma**; Areum Sohn[1]; Hyunsoo Kim[2]; Dongyoon Shin[3]; Youngsoo Kim[1, 4]; *[1]Department of Biomedical Sciences, Seoul National University College of Medicine, Seoul, South Korea; [2]Seoul National University Hospital, Seoul, Jongro-gu; [3]Seoul National University College of Medicine, Seoul, South Korea; [4]Department of Biomedical Engineering, Seoul National University College of Medicine, Seoul, Seoul, South Korea, Seoul, South Korea*

ThP 044 **Development and Qualification of a Sensitive and Robust Immunoaffinity UPLC-MRM MS Method for Quantitative Measurement of Angiopoietin-1 in Monkey Plasma**; Yuhuan Ji[1]; Joshuaine Toth[2]; Tammy Bigwarfe[2]; Chao Zheng[2]; Margit MacDougall[2]; Qian Li[1]; Jian Shi[1]; Vladimir Papov[2]; Peng Sun[2]; Ryan Fryer[2]; John Chen[1]; Laixin wang[1]; Chengjie Ji[1]; *[1]Novabioassays LLC, Woburn, MA; [2]Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT*

ThP 045 **Measuring Microbial Load in Unburned Tobacco using HPLC and Tandem Mass spectrometry**; Peter Kuklenyik[1]; Jacob B. Kimbrell[1, 2]; Robert Tyx[1]; Angel J. Rivera[1, 2]; Stephen Stanfill[1]; *[1]Centers for Disease Control, Atlanta, Georgia; [2]Oak Ridge Institute of Science & Education, WPAFB, OH*

ThP 046 **Streamlining Quantitative Assay Development Using Diagnostic Cluster Ions Native to Atmospheric Pressure Ionization**; RICHARD KING[1]; Susan Crathern[1]; Guille Metzler[1]; Lorin Bachmann[2]; carmen fernandez-metzler[1]; *[1]PharmaCadence Analytical Services, LLC, Hatfield, PA; [2]Virginia Commonwealth University, Richmond, VA*

ThP 047 **Development of a nonglycopeptide-based MRM strategy for screening of differential glycoproteins in hepatocellular carcinoma**; Weiqian Cao[1]; Bingyun Jiang[2]; Jiangming Huang[2]; Yi Wang[2]; Pengyuan Yang[2]; *[1]Fudan University, Shanghai, Shanghai; [2]Fudan University, Shanghai, China*

ThP 048 **Epitope fishing in digested biological samples**; Maren Levernæs[1]; Bassem Farhat[1]; Marianne Nordlund Broughton[2]; Léon Reubsaet[1]; Trine Grønhaug Halvorsen[1]; *[1]School of Pharmacy, University of Oslo, Oslo, Norway; [2]Department of Medical Biochemistry, Radiumhospitalet, Oslo University Hospital, Oslo, Norway*

ThP 049 **Comparison of Short-Chain Fatty Acids in Fecal vs. Plasma Samples using Gas Chromatography-Mass Spectrometry as Markers for the Gut Microbiome**; Vincent Windisch[1]; John A. Masucci[2]; Allen Xu[1]; *[1]Keystone Bioanalytical, North Wales, PA; [2]Janssen Research&Development, Spring House, PA*

ThP 050 **Highly Sensitive Mass Spectrometric Analysis of Tau Protein Isoforms in Human Cerebrospinal Fluid**; Yusaku Hioki[1]; Naoki Kaneko[1]; Ritsuko Yoda[1]; Sadanori Sekiya[1]; Shinichi Iwamoto[1]; Koichi Tanaka[1]; *[1]Shimadzu Corporation, Kyoto, Japan*

ThP 051 **MRM based Validation of Protein Biomarkers across Different Grades of Glioma Tissues**; Nikita Gahoi[1]; Saicharan Ghantasala[1]; Kishore Gollapalli[1]; Sanjeeva Srivastava[1]; Ajit Datar[2]; Rashi Kochhar[2]; Aliasgar Moiyadi[3]; Epari Sridhar[3]; *[1]Indian Institute of Technology Bombay, Mumbai, India; [2]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India; [3]Tata Memorial Hospital, Parel, Mumbai, India*

BIOMOLECULAR STRUCTURE ANALYSIS: CHEMICAL CROSSLINKING AND COVALENT LABELING II
052 - 072

ThP 052 **Improving Mass-Spectrometry Analysis of Protein Structures with Arginine-Specific Chemical Cross-linkers**; Alexander X. Jones[1]; Yong Cao[2]; Yue-He Ding[2]; Hui Tan[1]; Meng-Qiu Dong[2]; Xiaoguang Lei[1]; *[1]College of Chemistry, Peking University, Beijing, China; [2]National Institute of Biological Sciences, Beijing, Beijing, China*

ThP 053 **Optimization of Zero-Length Cross-linking Reaction Conditions Using Liquid Chromatography Mass Spectrometry to Probe Large Protein Complexes**; Pengyuan Liu[1]; Yekaterina Kori[1]; Sandra L. Harper[1]; Roland Rivera-Santiago[1]; David W. Speicher[1]; *[1]The Wistar Institute, Philadelphia, PA*

ThP 054 ***de novo* Protein Structure Determination by Short-Distance Crosslinking Constraint-Guided Discrete Molecular Dynamics Simulations**; Nicholas I. Brodie[1]; Jason J. Serpa[1]; Konstantin I. Popov[2]; Evgeniy V. Petrotchenko[1]; Nikolay V. Dokholyan[2]; Christoph H. Borchers[1, 3]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Dept. of Biochemistry and Biophysics, University of North Carolina School of Medicine, Chapel Hill, NC; [3]Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

ThP 055 **Novel Photo-Reactive Homo-Bifunctional Bis-Diazirine Short-Range Crosslinkers for Studying Protein Structure**; Nicholas I. Brodie[1]; Jason J. Serpa[1]; Evgeniy V. Petrotchenko[1]; Christoph H. Borchers[1, 2]; *[1]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; [2]Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada*

ThP 056 **NSLS-II XFP: X-ray Footprinting Beamline for *in vitro* and *in vivo* Structural Studies of Biological Macromolecules**; Jen Bohon[1, 2]; Don Abel[1]; Erik R. Farquhar[1]; John Toomey[1]; Michael Sullivan[1]; Mark R. Chance[1, 2, 3]; *[1]Center for Synchrotron Biosciences, Case Western Reserve University, Cleveland, OH; [2]Department of Nutrition, Case Western Reserve University, Cleveland, OH; [3]Center for Proteomics and Bioinformatics, Case Western Reserve University, Cleveland, OH*

ThP 057 **Kojak: Pipeline Developments and New Features for the Analysis of Chemically Cross-Linked Proteins**; Michael R. Hoopmann [1]; Alex Zelter[2]; Michael Riffle[2]; Luis Mendoza[1]; David Shteynberg[1]; Eric W. Deutsch[1]; Trisha N. Davis[2]; Robert L. Moritz[1]; *[1]Institute for Systems Biology, Seattle , WA; [2]University of Washington, Seattle, WA*

ThP 058 **Evaluation of a Series of Arginine-Specific Chemical Cross-Linkers for Mass Spectrometry Analysis of Proteins**; Alexander X. Jones[1]; Yong Cao[2]; Yue-He Ding[2]; Xiaoguang Lei[1]; Meng-Qiu Dong[2]; *[1]College of Chemistry, Peking University, Beijing, China; [2]National Institute of Biological Sciences, Beijing, Beijing, China*

ThP 059 **Label-free Quantitative Cross-Linking for Conformational Analysis by SIM-XL**; Fabio C Gozzo[1]; Luana Oliveira[1]; Allan JR Ferrari[1]; Diogo Borges Lima[2]; Paulo Costa Carvalho[3]; *[1]University of Campinas, Campinas, SP; [2]Institut Pasteur, Paris; [3]Carlos Chagas Institute - Fiocruz, Curitiba, Brazil*

ThP 060 **OpenProXL: a Fast and Versatile XL-MS Identification Tool**; Eugen Netz[1]; Timo Sachsenberg[2]; Christian Johannes Gloeckner[3]; Oliver Kohlbacher[1, 2]; *[1]Max Planck Institute for Developmental Biology, Tübingen, Germany; [2]Universität Tübingen, Tübingen, Germany; [3]German Center for Neurodegenerative Diseases Tübingen, Tübingen, Germany*

ThP 061 **Hydroxyl Radical Footprinting with PLIMB (Plasma-Induced Modification of Biomolecules): A New Tool for Structural Mass Spectrometry**; Benjamin B. Minkoff[1]; Joshua Blatz[1]; Daniel Benjamin[1]; Faraz Choudhury[1]; J. Leon Shohet[1]; Michael R. Sussman[1]; *[1]University of Wisconsin-Madison, Madison, WI*

ThP 062 **Fast Photochemical Oxidation of Proteins Coupled with Ion Mobility-Mass Spectrometry to Characterize Structural Differences between Protein Conformers**; Emily Hart[1]; Daniel J. Deredge[1]; Lisa M. Jones[1]; *[1]University of Maryland School of Pharmacy, Baltimore, MD*

ThP 063 **Perfluoroalkyl Radicals for Footprinting Soluble and Membrane Proteins**; Ming Cheng[1]; Michael L. Gross[2]; *[1]Washington University, St.Louis, MO; [2]Washington University, St. Louis, MO*

ThP 064 **High Resolution Mapping of Drug Binding Site Using Hydroxyl Radical Footprinting**; Janna Kiselar[1]; Stephanie Stanford[2, 3]; Alexander E Aleshin[4]; Sichun Yang[1]; Vida Zhang[2, 3]; Robert J Ardecky[5]; Gregory W Cadwell[4]; Jinghua Yu[5]; Laurie A Bankston[4]; Robert C Liddington[4]; Anthony Pinkerton[5]; Mark R Cance[1]; Nunzio Bottini[2, 3]; *[1]Department of Nutrition, Case Western Reserve Univ, Cleveland, OH; [2]Division of Cellular Biology, La Jolla Institute for Allergy and Immunology, La Jolla, CA; [3]Department of Medicine, University of California, San Diego, CA; [4]Infectious and Inflammatory Disease Center, Sanford Burnham Prebys Medical Discovery Institute, La Jolla, CA; [5]Conrad Prebys Center for Chemical Genomics, Sanford Burnham Prebys Medical Discovery Institute, La Jolla, CA*

ThP 065 **Amino Acid Analysis of Carbene Footprinting by Enzymatic Hydrolysis and GC-MS**; Bojie Zhang[1]; Daryl Giblin[1]; Ming Cheng[1]; Michael L. Gross[1]; *[1]Washington University in St. Louis, St. Louis, MO*

ThP 066 **Structural Elucidation *via* Automated Analysis of Complex Protein Crosslinking Data**; Allis S. Chien[1]; Eric Carlson[2]; Marshall W. Bern[2]; Wilfred H. Tang[2]; Christopher Becker[2]; Ryan D. Leib[1]; Christopher M. Adams[1]; *[1]Vincent Coates Foundation Mass Spectrometry Laboratory, Stanford University, Stanford, CA; [2]Protein Metrics Inc., San Carlos, CA*

ThP 067 **High Confidence Identification of Crosslinked Peptides Using a Dual Cleavable Crosslinker (DUCCT) with Enrichment Functionality**; Jayanta Kishor Chakrabarty[1]; Abu Hena M Kamal[2]; Zixiang Fang[2]; Saiful M. Chowdhury[2]; *[1]University of Texas, Arlington, Arlington, TX; [2]University of Texas at Arlington, Arlington, TX*

ThP 068 **Carbonate Radical Anion as a new reagent for Fast Photochemical Oxidation of Proteins**; Mengru Zhang[1]; Michael L. Gross[2]; *[1], St. Louis, Missouri; [2]WUSTL, St. Louis, MO*

ThP 069 **Enrichment Strategies for Improvement of Mass Spec Analysis of Chemical Cross-Linked Peptides**; Rosa Viner[1]; Ryan Bomgarden[2]; Kratika Singhal[2]; Sergei Snovida[2]; Craig Gutierrez[3]; Lan Huang[3]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Rockford, IL; [3]UC Irvine Department of Physiology & Biophysics, Irvine, CA*

ThP 070 **Chemical Cross-Linking (CXL) Products Analysed by LC-Ion Mobility (IM)-MS/MS**; Denise P Tran[1]; Paul J Trim[2]; Marten F Snel[2]; Tara L Pukala[1]; *[1]The University of Adelaide, Adelaide, Australia; [2]South Australian Health and Medical Research Institute, Adelaide, Australia*

ThP 071 **MS-Fold: Protein Structure Prediction Guided by Covalent Labeling Mass Spectrometry Data**; Melanie L Aprahamian[1]; Samantha H Hinckley[1]; Vicki H. Wysocki[1]; Steffen Lindert[1]; *[1]Ohio State University, Columbus, OH*

ThP 072 **Cross-Linking Visualization and Analysis Using CX-Circos 2**; Junjie Wang[1]; Yi Shi[1]; Brian T Chait[1]; *[1]Rockefeller University, New York, NY*

CLINICAL ANALYSIS II
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ThP 073 **A High Sensitivity LC/MS/MS Method for Quantitative Analysis of Eight Antifungal Drugs in Human Serum**; Tze Peng Lim[1]; Yuan Cao[2]; Shao Hua Chia[2]; Si Xuan Tan[1]; Zhao Qi Zhan[2]; Jie Xing[2]; *[1]Pharmacy, Singapore General Hospital, Singapore, Singapore; [2]Application Development & Support Centre, Shimadzu (Asia Pacific) Pte Ltd, 79 Science Park Drive #02-01/08,, Singapore, Singapore*

ThP 074 **Direct Injection of Antiretroviral Drugs in Highly Organic Protein-Precipitated Human Plasma by LC-MS/MS**; Frances Carroll[1]; Justin Steimling[1]; Susan Steinike[1]; *[1]Restek Corporation, Bellefonte, PA*

ThP 075 **Quantification of 3α and 3β epimers of 25-Hydroxyvitamin D3 in DBS Using Artificial Whole Blood Calibration and Chemical Derivatization**; Miriam Müller[1]; Caroline Stokes[1]; Dietrich Volmer [1]; *[1]Saarland University, Saarbrücken*

ThP 076 **LC-MS-MS Quantitative Analysis of Thyroid Hormones and Metabolites in Serum for Research Use**; Rory M Doyle; *Thermo Fisher Scientific, Somerset, NJ*

ThP 077 **Rapid Quantification of Endogenous Cholesterol in Human Serum on Filter Paper Using Direct Analysis in Real Time Mass Spectrometry (pDART-MS)**; Hua-Yi Hsieh[1]; Li-Hua Li[2, 3]; Ren-Yu Hsu[1]; Ying-Chen Huang[1]; Wei-Fong Kao[4, 5]; Cheng-Chih Hsu[1]; *[1]Department of Chemistry, National Taiwan University, Taipei, Taiwan; [2]Department of Pathology and Laboratory Medicine, Taipei Veterans General Hospital, Taipei, Taiwan; [3]School of Medical Laboratory Science and Biotechnology, Taipei Medical University, Taipei, Taiwan; [4]Chief, Department of Emergency & Critical Care Medicine, Taipei Medical University Hospital, Taipei, Taiwan; [5]Department of Emergency medicine, School of Medicine, College of Medicine, Taipei Medical University, Taipei, Taiwan*

ThP 078 **Enzyme Activities in Six Lysosomal Storage Diseases in Japanese Neonates Determined by LC-MS/MS**; Ryuichi Mashima[1]; Motomichi Kosuga[1]; Torayuki Okuyama[1]; *[1]National Center for Child Health and Development, Setagaya-ku, Japan*

ThP 079 **Quantitative Analysis of β-Lactam Antibiotics in Human Plasma by High Sensitivity LC/MS/MS Method**; Daryl Kim Hor Hee[1]; Zhi Wei Edwin Ting[2]; Lawrence Soon-U Lee[1]; Jie Xing[3]; Kelvin Loh Shun Cheng[4]; Zhaoqi Zhan[3]; *[1]Clinical Analysis Centre, Department of Medicine Research Laboratories, National University of Singapore, Singapore, Singapore; [2]Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore; [3]Shimadzu Asia Pacific, Singapore, Singapore; [4]School of Physical and Mathematical Science, Nanyang Technical University, Singapore, Singapore*

ThP 080 **Multiplexed Quantification of Anti-Tuberculosis (anti-TB) Drugs in Plasma and Tissue *via* LC-MS/MS Analysis**; Pamela Hummert[1]; Mark Marzinke[2]; *[1]Johns Hopkins University, Baltimore, MD; [2]Johns Hopkins University, Baltimore, MD*

ThP 081 **Multiplex Tandem Mass Spectrometry Assays of Six Protein and Glycosaminoglycan Degrading Lysosomal Enzymes in Dried Blood Spots for Newborn Screening**; Frantisek Turecek[1]; Yang Liu[1]; Fan Yi[1]; Ronald Scott[1]; Michael H Gelb[1]; *[1]University of Washington, Seattle, WA*

ThP 082 **New approaches for Enzyme Replacement Therapy of Lysosomal Diseases byIdentification and Affinity Quantification of Antibody Epitopes** ; Michael Przybylski[1]; Zdenek Kukacka[1]; Stefan Maeser[1]; Fabio Borri[1, 2]; Lorenzo Altamore[2]; Julia Hennermann[3]; Anna Maria Papini[2]; *[1]Steinbeis Centre Biopolymer Analysis and Biomedical Mass Spectrometry, Ruesselsheim am Main, Germany; [2]Department of Peptide Chemistry and Biology, University of Florence, Florence, Italy; [3]Unimedizin, Villa Metabolica, Universität Mainz, Mainz, Germany*

ThP 083 **Improving Accuracy of Reference Measurements for Serum 25-Hydroxyvitamin D Metabolites by Switching from Solvent- to Serum-Based Calibration** ; Ekaterina Mineva[1]; Rosemary Schleicher[1]; Shahzad Momin[1]; Khin Maw[1]; *[1]Centers for Disease Control and Prevention, Atlanta, Ga*

ThP 084 **Evaluation of Blood Lysis Procedures prior to Automated Sample Preparation for Immunosuppressant Assay by LC-MS/MS**; Eishi Imoto[1]; Mikael Levi[1]; Atsuhiko Toyama[1]; Daisuke Kawakami[2]; Jun Watanabe[1]; *[1]Shimadzu Corporation., MS BU, Kyoto, Japan; [2]Shimadzu, Kyoto, Japan*

ThP 085 **Detection and Quantification of Carbohydrate Deficient Transferrin by MALDI-Compatible Protein Chips Prepared by Ambient Ion Soft Landing**; Petra Darebna[1, 2]; Petr Pompach[1, 2, 3]; Michal Rosulek[1, 2]; Michael Volny[1, 3]; Petr Novak[1, 2, 3]; *[1]BIOCEV, Institute of Microbiology of the CAS, v.v.i., Vestec, Czech Republic; [2]Faculty of Science, Charles University, Prague, Czech Republic; [3]AffiPro s.r.o., Mratin, Czech Republic*

ThP 086 **Fully Automated Platform for Sensitive Determination of Immunosuppressant Drugs in Whole Blood, Using High Quality Internal Standardization**; Aurore Jaffuel[1]; Marc Fernandez[1]; Alban Huteau[1]; *[1]Shimadzu France, Paris, France*

ThP 087 **Evaluation of Interaction of Hop Botanical Dietary Supplements with Drug Metabolism in Women**; Luying Chen[1]; Alyssa Tonsing-Carter[1]; Richard van Breemen[1]; *[1]University of Illinois College of Pharmacy, Chicago, IL*

ThP 088 **Single Assay Measurement of Aldosterone-to-Renin Ratio by Online SPE-UHPLC-MS/MS**; Mikael Levi[1]; Nicola Gray[2]; Oneal Joseph[3]; Ichiro Hirano[1]; *[1]Shimadzu Corp., MS BU, Kyoto, Japan; [2]Shimadzu UK Limited, Milton Keynes, UK; [3]Health Services Laboratory, London, UK*

ThP 089 **Quantitative and Rapid Carbapenem Susceptibility Test for Bacteria Based on LDI-TOF MS**; Jong Min Park[1]; Joo-Yoon Noh[1]; Mira Kim[1]; Moon-Ju Kim[1]; Jae-Chul Pyun[1]; *[1]Yonsei University, Seoul, South Korea*

ThP 090 **Fully Automated Platform for Determination of Tricyclic Antidepressant in Serum**; Davide Vecchietti[1]; Claudio Ghilardi[2]; Katharina Kern[3]; Stéphane Moreau[4]; Isabel Cabruja[2]; *[1]Shimadzu, Milan, Lombardy; [2]Shimadzu Italy, Milan, Italy; [3]Recipe Chemicals + Instruments GmbH, Munich, Germany; [4]Shimadzu Europe GmbH, Duisburg, Germany*

ThP 091 **Comparison of FIA and On-Column LC-MS/MS Method to Measure Simultaneously ABG, ASM, GAA, GALC, GLA and IDUA Activities**; Misa Tanaka[1]; Osamu Ohara[2]; Jun Watanabe[1]; Toshikazu Minohata[1]; Eishi Imoto[1]; Junichi Masuda[1]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Kazusa DNA Research Institute, Kisarazu, Japan*

ThP 092 **LC-MS-MS Quantitative Analysis of Folic Acid, its Metabolites and Derivatives in Serum for Research Use**; Rory M Doyle[1]; Catherine Riley[1]; *[1]Thermo Fisher Scientific, Somerset, NJ*

ThP 093 **Fully Automated Online Sample Preparation AND Quantification of Amiodarone from Whole Blood Using CLAM-LC-MS/MS**; Christian Bunse[1]; Lars Kröner[2]; *[1]Shimadzu Deutschland GmbH, Duisburg, Germany; [2]Labor Dr. Wisplinghoff, Cologne, Germany*

ThP 094 **Detection of Vitamin D Metabolites Based on Dried Blood Spot Sampling in Combination with LC/MS/MS High-Throughput Analysis**; Konrad Piotr Kowalski[1, 2]; Tomasz Bienkowski[1, 2]; *[1]Masdiag Sp. z o.o., Warszawa, Mazowieckie; [2]MS Ekspert Sp. z o.o., Gdańsk, Poland*

ThP 095 **Determination of Plasma DHA Using UPLC-MS/MS in APRT Deficient Patients with Ocular Manifestations**; Margret Thorsteinsdottir[1, 2]; Unnur A. Thorsteinsdóttir[1, 2]; Hrafnhildur L. Runolfsdottir[1, 3]; Finnur F. Eiriksson[1, 2]; Vidar O. Edvardsson[1, 3]; Runolfur Palsson[1, 3]; *[1]University of Iceland, Reykjavik, Iceland; [2]ArcticMass, Reykjavík, Iceland; [3]Landspitali – The National University Hospital of Iceland, Reykjavik, Iceland*

ThP 096 **UHPLC-MS/MS quantitative analysis of estrogen metabolites in human serum**; Alan Wong[1]; Lingyi Huang[1]; Shuai Wang[1]; Caitlin Howell[1]; Judy L. Bolton[1]; Richard B. van Breemen[1]; *[1]University of Illinois at Chicago, Chicago, IL*

ThP 097 **High-sensitivity, high-throughput quantitation of catecholamines in plasma by Automatable Derivatization and SPE Coupled to LC-MS/MS for Clinical Research**; Atsuhiko Toyama[1]; Mikael Levi[1]; Ichiro Hirano[1]; Jun Watanabe[1]; *[1]Shimadzu Corporation, Kyoto, Japan*

ThP 098 **Monitoring Simvastatin Metabolism using LC/MS as a Diagnostic Tool for Celiac Disease Activity**; Jennifer Sealey Voyksner[1]; Josesph A Murray[2]; Jack Syage[3]; Chaitan khosla[4]; *[1]ImmunogenX, Durham, NC; [2]Mayo Clinic, Rochester, MN; [3]ImmunogenX, Newport Beach, California; [4]Stanford University, Stanford, CA*

ThP 099 **Quantitation of Plasma Metanephrine and Normetanephrine by Derivatization Using an Integrated LC-MS/MS Analyzer Equipped with Fully-Automated Sample Preparation Device**; Taku Tsukamoto[1]; Daisuke Kawakami[1]; Atsuhiko Toyama[1]; *[1]Shimadzu Corporation, Kyoto, Japan*

ThP 100 **Fast and Sensitive Method for the LCMS Analysis of Vitamin D**; Tim Schlabach[1]; Jinhee Kim[1]; *[1]Novilytic LLC, West Lafayette, IN*

ThP 101 **Improvement of Stability and Reproducibility of Standard Solutions to Guarantee Robust and Reliable Data in LC-MS Analyses Using READYBEADS**; Jordane Biarc[1]; Quentin Enjalbert[1]; Chloe Bardet[1]; Christelle Jacquet[1]; Lou Van Poeck[1]; Tanguy Fortin[1]; *[1]ANAQUANT, Villeurbanne, France*

ThP 102 **Quantitative Determination of Free Hormone Fraction *via* Biocompatible Solid Phase Microextraction (BioSPME)**; Sara Smith[1]; Candace Price[2]; Emily Barrey[2]; Craig Aurand[2]; Dave Bell[2]; *[1]Millipore Sigma, Bellefonte, PA; [2]MilliporeSigma, Bellefonte, PA*

ThP 103 **Simple and Robust LC-MS/MS Method of the Alcohol Biomarker Phosphatidylethanol (PEth) in Whole Blood using Luna Omega Polar C18 Column** ; Xianrong (Jenny) Wei[1]; Sean Orlowicz[1]; *[1]Phenomenex, Inc., Torrance, CA*

DISEASE BIOMARKERS
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ThP 105 **Integrated Metabolomics and Metallomics Analysis in Acute Coronary Syndrome Patients**; SAM LI[1]; Xuejiao Yin[1]; Leonardo Pinto de Carvalho[1]; Mark Chan[1]; *[1]National University of Singapore, Singapore, Singapore*

ThP 106 **Quantitative Proteomics of Murine Exosomes Following Aerosol Exposure to 4,4'-Methylene Diphenyl Diisocyanate**; Brandon F. Law[1]; Chen-Chung Lin[1]; Paul D. Siegel[1]; Justin M. Hettick[1]; *[1]NIOSH, Morgantown, WV*

ThP 107 **Inhaled 4,4'-Methylene Diphenyldiisocyanate Particulates Haptenate Serum Albumin at Lys535 in Murine Bronchoalveolar Lavage Fluid**; Justin M. Hettick[1]; Brandon F. Law[1]; Chen-Chung Lin[1]; Paul D. Siegel[1]; *[1]NIOSH, Morgantown, WV*

ThP 108 **A Comprehensive Protein Biomarker Study of Cerebrospinal Fluid from Smith-Lemli-Optiz Patients**; Alfred L. Yergey[1]; Stephanie M. Cologna[2]; Melissa R. Pergande[2]; Matthew T. Olson[3]; Peter S. Backlund[1]; Christopher A. Wassif[1]; Brian C. Searle[4]; Jacqueline A. Picache[1, 5]; Kathryn R. Burkert[1]; Vadiraja Bhat[6]; Carol Haney-Ball[6]; Forbes D. Porter[1]; *[1]National Institutes of Health, Bethesda, MD; [2]University of Illinois at Chicago, Chicago, IL; [3]Johns Hopkins University, Baltimore, MD; [4]Proteome Software, Portland, OR; [5]Vanderbilt University, Nashville, TN; [6]Agilent Technologies, Wilmington, DE*

ThP 109 **Tegumentray Leishmaniasis Investigated by DESI Imaging and Profile**; Fernanda Negrão[1]; Daniele F. de O. Rocha[1]; Célio F. F. Angolini[1]; Caroline F. Jaeeger[1]; Daniel R. Abánades[1]; Selma Giorgio[1]; Marcos N. Eberlin[1]; *[1]UNICAMP, Campinas, SP*

ThP 110 **Discovering Novel Immunotherapy Targets for Multiple Myeloma with Cell Surface Capture Technology and Parallel Reaction Monitoring Mass Spectrometry**; Nathan J. Schuld[1]; Theodore R. Keppel[1]; Ensaf M. Hujaily[1]; Parameswaran Hari[1]; Jeffrey A. Medin[1]; Rebekah L. Gundry[1]; *[1]Medical College of Wisconsin, Milwaukee, WI*

ThP 111 **Novel Biomarkers for Respiratory Diseases Discovered by Secondary Electrospray Ionization – High Resolution Mass Spectrometry**; Nora Nowak[1]; Martin T. Gaugg[1]; Lukas Bregy[1]; Tobias Bruderer[1]; Pablo Martinez-Lozano Sinues[1]; Alexander Möller[2]; Malcolm Kohler[3]; Renato Zenobi[4]; *[1]ETH Zurich, Department of Chemistry and Applied Biosciences, Zurich, Switzerland; [2]Kinderspital Zürich, Zurich, Switzerland; [3]University Hospital Zurich, Zurich, Switzerland; [4]ETH Zurich, Zurich*

ThP 112 **Localization of Disease Biomarkers in Juvenile Cystic Kidney Using Tissue Mass Spectrometry Imaging**; Cristina I. Silvescu[1]; Hanlan Liu[1]; Thomas Natoli[2]; Laurie Smith[2]; Mandy Cromwell[3]; Dinesh Bangari[4]; Susan Ryan[4]; Petra Oliva[5]; Lilu Guo[6]; Alla Kloss[6]; Thomas O'Shea[1]; Walter Korfmacher[1]; *[1]Drug Metabolism and Pharmacokinetics, Sanofi, Waltham, MA; [2]Rare Renal and Bone Disease Research, Sanofi, Framingham, MA; [3]Rare Disease Pharmacology, Sanofi, Waltham, MA; [4]Pathology, Sanofi, Framingham, MA; [5]Biological Mass Spectrometry, Sanofi, Framingham, MA; [6]Analytical Research and Development, Sanofi, Waltham, MA*

ThP 113 **Ratiometric Mass Spectrometry Determination of GALE Activity**; Ruth Gordillo[1]; Yi Zhu[1]; Preethi Csudae[1]; Benjamin J. Figard[2]; Jone Garate[3]; Duyen Do[1]; Philipp E Scherer[1]; *[1]Touchstone Diabetes Center, Department of Internal Medicine, Dallas, Texas; [2]Shimadzu Scientific Instruments, Columbia, MD; [3]Department of Physical Chemistry, University of the Basque Country, Leioa, Afghanistan*

ThP 114 **Targeted Sphingolipid Profiling of Tumor and Plasma Samples in Murine Lung Carcinoma Model Revealing the Mechanism of Doxorubicin**; Ujjaini Dasgupta[1]; Nihal Medatwal[2]; Avinash Bajaj[2]; Dipanakar Malakar[3]; Manoj Pillai[3]; Sandeep Kumar[2]; *[1], Gurgaon, Haryana; [2]Regional Center for Biotechnology, Faridabad, India; [3]SCIEX, 121, Udyog Vihar, Phase IV., Gurgaon, India*

ThP 115 **Quantitative Analysis of ALS/FTD C9ORF72 Protein Isoforms in Cynomolgus Monkey Brain Tissue by Nano-LC and Triple Quadrupole Mass Spectrometer** ; Rong-Fang Gu[1]; Alexander McCampbell[2]; Mia M. Rushe[2]; Peter Juhasz[2]; Ru Wei[2]; *[1]Biogen, Cambridge, MA; [2]Biogen, Cambridge, MA*

ThP 116 **Identification and functional assay of missing proteins in cancer research**; Yu-Chang Tyan[1]; Ming-Hui Yang[1]; Po-Chiao Huang[1]; *[1]Kaohsiung Medical University, Kaohsiung, Taiwan*

ThP 117 **Large-Scale Analysis of Protein Conformational Changes for Biomarker Discovery in Breast Cancer**; Fang Liu[1]; Michael C. Fitzgerald[1]; *[1]Duke University, Durham, NC*

ThP 118 **Proteomic Analysis of Right-Side and Left-Side Colon Cancer Tumors**; Katelyn Ludwig[1]; Heinz-Josef Lenz[2]; Amanda B. Hummon[1]; *[1]University of Notre Dame, Notre Dame, IN; [2]University of Southern California, Los Angeles, CA*

ThP 119 **Enrichment of Hydrophobic Endogenous Peptides in Urine from Patients with Severe Preeclampsia by Mesoporous Silica Chips**; Hongwu Jing[1]; Irina A. Buhimschi[2]; Guomao Zhao[2]; Megan Locke[2]; Sten Heinze[2]; Jason Sakamoto[3]; Catalin S. Buhimschi[4]; Vicki H. Wysocki[1]; *[1]The Ohio State University, Columbus, OH; [2]Center for Perinatal Research, The Research Institute at Nationwide Children's Hospital, Columbus, OH; [3]NanoMedical Systems, Houston, TX; [4]Department of Obstetrics and Gynecology, The Ohio State University, Columbus, OH*

ThP 120 **Experiment Design and Quality Control for a Large Scale Cancer Proteomics Project: A How-To Guide**; Bin Fang[1]; Victoria Izumi[1]; Paul A Stewart[1]; Robbert JC Slebos[1]; Eric A Welsh[1]; Ling Cen[1]; Yonghong Zhang[1]; Zhihua Chen[1]; Chia-Ho Cheng[1]; Fredrik Pettersson[1]; Anders Berglund[1]; Guolin Zhang[1]; Sean Yoder[1]; Katherine Fellows[1]; Ann Y. Chen[1]; Jamie K Teer[1]; Steven Eschrich[1]; John Koomen[1]; Eric B Haura[1]; *[1]H. Lee Moffitt Cancer Center, Tampa, FL*

ThP 121 **Affinity Capture MRM Analysis of Molecular Forms of B-type Natriuretic Peptide**; Billy J Molloy[1]; James Langridge[1]; Leong L Ng[2]; Thomas Walther[3, 4]; Johannes PC Vissers[1]; Donald JL Jones[2, 5]; Toru Suzuki[2, 6]; *[1]Waters corporation, Wilmslow, UK; [2]Department of Cardiovascular Sciences, University of Leicester, NIHR Leicester Cardiovascular Biomedical Research Unit, Glenfield Hospital, Leicester, UK; [3]Department of Pharmacology and Therapeutics, University College Cork, Cork, Ireland; [4]Institute of Medical Biochemistry and Molecular Biology, University Medicine Greifswald, Greifswald, Germany; [5]Department of Cancer Studies, RKCSB, University of Leicester, Leicester, UK; [6]Jichi Medical University, Tochigi, Japan*

ThP 122 **Investigating the Metabolic Links between Insulin Dysregulation, Obesity, and Laminitis in Welsh Ponies via Mass Spectrometry and Statistical Models**; Kevin Murray[1]; Sarah Jacob[2]; Ray Geor[3]; Elaine Norton[1]; Nichol Schultz[1]; Molly McCue[1]; *[1]University of Minnesota, Minneapolis, Minnesota; [2]Michigan State University, Lansing, MI; [3]Massey University College of Science, Palmerston North, New Zealand*

ThP 123 **Proteomic Analysis of Exosomes Derived Alzheimer's Disease Brain Tissue**; Manveen K Sethi[1]; Annina DeLeo[2]; Tsuneya Ikezu[2]; Joseph Zaia[1]; *[1]Center for Biomedical Mass Spectrometry, Department of Biochemistry, Boston University School of Medicine, Boston, MA; [2]Department of Pharmacology & Experimental Therapeutics, Boston University School of Medicine, Boston, MA*

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ThP 125 **Application of a Comparative Lipidomic Approach to Distinguish Pathogenic Staphylococci**; Naren Gajenthra Kumar[1]; Kim Ekroos[2]; Kimberly Jefferson[1]; Dayanjan S Wijesinghe[1]; *[1]Virginia Commonwealth University, Richmond, VA; [2]Lipidomics Consulting Ltd., Irisviksvägen, Finland*

ThP 126 **A Proteomic Fingerprint of Hormone-Induced Lower Urinary Tract Dysfunction in Mice**; Samuel Thomas[1]; Ling Hao[2]; Dustin Frost[2]; Paul Marker[2]; William Ricke[1, 3]; Lingjun Li[1, 2]; *[1]Molecular and Environmental Toxicology Center, University of Wisconsin-Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [3]Department of Urology, University of Wisconsin-Madison, Madison, WI*

ThP 127 **Proteomic Profiling of Plasma, iPSC, 3D Neuron, and Brain Tissue from Alzheimer Patients Using LC-MS/MS**; Mei Chen[1]; Han-Kyu Lee[1]; Peter Morin[1]; John M Wells[1]; Eugene B Hanlon[1]; Nicole Daniels[1]; Lauren Moo[1]; Thor Stein[1, 2]; Weiming Xia[1, 3]; *[1]Edith Nourse Rogers Memorial Veterans Hospital, Bedford, MA; [2]Boston University School of Medicine, Boston, MA; [3]Boston University School of Medicine, Boston, MA*

ThP 128 **Quantitative Analysis of PZP in Serum: Validation of a Risk Factor for Alzheimer's Disease**; Diana Nijholt[1]; Christoph Stingl[1]; Peter Koudstaal[1]; Peter Sillevis Smitt[1]; Arfan M. Ikram[1]; Theo M. Luider[1]; *[1]Erasmus MC, Rotterdam, Netherlands*

ThP 129 **Mass Spectrometry- based Proteomics of Human Breast Milk for Breast Cancer Biomarker Discovery**; Roshanak Aslebagh[1]; Devika Channaveerappa[1]; Kathleen F. Arcaro[2]; Costel C. Darie[1]; *[1]Clarkson University, Potsdam, NY; [2]University of Massachusetts, Amherst, Amherst, MA*

ThP 130 **Predicting Childhood Asthma Using Urine Proteomics**; Tess Kelly[1]; Brooke Thompson[1]; Paulos Chumala[1]; Oluwafemi Oluwole[1]; Anna Afanasieva[1]; Donna Rennie[2]; Joshua Lawson[1]; George S. Katselis[1]; *[1]CCHSA/ Department of Medicine, College of Medicine, University of Saskatchewan, Saskatoon, SK, Canada; [2]CCHSA and College of Nursing, University of Saskatchewan, Saskatoon, SK, Canada*

ThP 131 **The Role of Free Fatty Acids in Pulmonary Fibrosis**; Hyun Ju Yoo; *Biomedical Research Center, Asan Institute for Life Sciences, Asan Medical Center, Seoul, South Korea*

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ThP 133 **PaperSpray Technology for the Study of Selective High Affinity Ligands (SHALs) and their Metabolites**; Maria C. Prieto Conaway[1]; Kerry M Hassell[2]; Rodney Balhorn[3]; *[1]Thermo Fisher Scientific, San Jose , CA; [2]Thermo Fisher Scientific, Somerset, NJ; [3]SHAL Technologies, Inc., Livermore, CA*

ThP 134 **Paper Spray Mass Spectrometry for Screening of Antifungal Drugs from Plasma Samples**; Christine Skaggs; *, Indianapolis, IN*

ThP 135 **Post-mortem Drug Screening Using Paper Spray MS on a Q-Orbitrap Mass Spectrometer**; Josiah McKenna[1]; Rachel Potter[1]; Nicholas Manicke[1]; *[1]IUPUI, Indianapolis, IN*

ThP 136 **An Integrated Dried Blood Spot (DBS) Collection, Storage and Extraction Device— Towards an Automated Work Flow for Capillary Blood Samples**; Ricardo Neto[1, 2]; Wei Boon Hon[1, 3]; Hans-Jürgen Wirth[1, 3]; Andrew Gooley[1, 3]; Florian Lapierre[1, 4]; Robert Shellie[1, 3]; R. Dario Arrua[1, 2]; Emily F., Hilder[1, 2]; *[1]ARC Training Centre for Portable Analytical Separation Technologies, 7 Argent Place, Ringwood, 3134, Australia; [2]University of South Australia, Mawson Lakes Campus, Adelaide 5001, Australia; [3]Trajan Scientific and Medical, 7 Argent Place, Ringwood, 3134, Australia; [4]University of Tasmania, Sandy Bay, Hobart,7005, Australia*

ThP 137 **Large Molecule Application of Volumetric Absorptive Microsampling for Single-Rodent PK Profiling of Exenatide Determined by LC-MRM**; Jeff Plomley[1]; Daniel Villeneuve[1]; Mingluan Chen[1]; Kevork Mekhssian[1]; Anahita Keyhani[1]; Olivier Didur[2]; William Ruddock[2]; Luca Genovesi[1]; *[1]Algorithme Pharma an Altasciences company, Laval, QC, Canada; [2]ITR Laboratories, Montreal, QC, Canada*

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ThP 139 **LC-MS/MS Combined with Single-Step Extraction Method for the Determination of Nicotine and Cotinine Metabolite in Rat Plasma**; Changyu Quang[1]; Kathleen J. McQuate[1]; Jennifer L. Simko[1]; William C. Nethero[1]; Liam B. Moran[1]; Elizabeth A. Groeber[1]; *[1]Charles River Labs, Ashland, OH*

ThP 140 **Hematocrit Effect: Any Influence in Plasmas Sample Analysis or just a DBS Concern?**; Serge Auger[1]; Jean Lacoursiere[1]; Pierre Picard[1]; *[1]Phytronix Technologies, Quebec, QC, Canada*

ThP 141 **In Tips Micro-Sampling Comparison with Standard Volume Plasma Protein Precipitation with an On-Line Sample Preparation System**; Kimiaka-Chantal Guerard[1]; Sylvain Latarte[1]; Serge Auger[2]; Pierre Picard[2]; *[1]Phytronix Instruments, Boisbriand, QC, Canada; [2]Phytronix Technologies, Québec, QC, Canada*

ThP 142 **Dried-Blood-Spot Sampling-Device that Solves the Hematocrit-Problem, is Patient Friendly, has Timestamp Functionality, and is Amenable to Complex & Automated Processing**; Lars Liepold; *AmpleSample, Minneapolis, MN*

ThP 143 **Detection of Growth Promoting Agents in Equine Dried Blood Spots Using Liquid Chromatography - Tandem Mass Spectrometry**; Benjamin C Moeller[1]; Zicheng Yang[2]; Amel J Clifford[1]; Scott D Stanley[1]; *[1]University of California, Davis, School of Veterinary Medicine, KL Maddy Equine Analytical Chemistry Laboratory, Davis, CA; [2]Bruker Daltonics, Fremont, CA*

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ThP 147 **Low Level Quantification of NDMA and Non-Targeted Contaminants Screening in Drinking Water Using GC-Orbitrap-Mass Spectrometry**; Dan Quinn; *Thermo Fisher Scientific, Chardon , OH*

ThP 148 **Expanding Horizons in Real Time Analysis: Dual Polarity SIFT-MS**; Murray J Mcewan[1]; Thomas I McKellar[2]; Vaughan S Langford[2]; David Hera[2]; Daniel B Milligan[2];

[1]University of Canterbury, Christchurch, Canterbury; [2]Syft Technologies Ltd, Christchurch, New Zealand

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ThP 150 **Screening for Water Contaminants by All-Ion Fragmentation in Rhine River Samples**; Sylvain Merel[1]; Gina Di Napoli-Davis[1]; Christian Zwiener[1]; [1]Universität Tübingen, Tübingen, Germany

ThP 151 **A Sensitive and Automation Approach Using large Volume Injection System Couple with LC-MS/MS to Analyze Perfluorinated Compounds in Environmental Samples**; Wen-Yen Lee[1]; Dai-Yong Huang[2]; Yanan Yang[3]; Shan-An Chan[1]; [1]Agilent Technologies Inc., Taipei, Taiwan; [2]Agilent Technologies Ltd. Hong Kong, Hong Kong, Hong Kong; [3]Agilent Technologies Inc., Santa Clara, CA

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ThP 153 **Analysis of Dioxins, Furans and Polychlorinated Biphenyls in Sediments and Fish Using the Novel 7250 High-Resolution GC/Q-TOF**; Peter Haglund[1]; Sofia Nieto[2]; Nathan Eno[2]; [1]Umeå University, Umeå, Sweden; [2]Agilent Technologies, Inc., Santa Clara, CA

ThP 154 **Extraction and Analysis of Poly Brominated Diphenyl Ether in Aqueous Samples Using EPA 1614**; Rashid Juma[1]; Rudolf Addink[1]; [1]Toxic Report, Watertown, MA

ThP 155 **Identification of Halogenated Disinfection Byproducts of Nonylphenol in Chlorinated Wastewater Effluent Using a Novel High Resolution GC/Q-TOF**; Christiane Hoppe-Jones[1]; Sofia Nieto[2]; Nathan Eno[2]; Craig Marvin[3]; Shane Snyder[1]; [1]University of Arizona, Tucson, AZ; [2]Agilent Technologies, Inc., Santa Clara, CA; [3]Agilent Technologies, Inc., Wilmington, DE

ThP 156 **Application of a Non-Targeted Screening Workflow to Identify Toxic Contaminants in Waste Water Effluent**; Bernadette Vogler[1]; Christian Götz[2]; Bernd Kobler[3]; Heinz Singer[1]; [1]EAWAG, Dübendorf, ZH; [2]Envilab AG, Zofingen, Switzerland; [3]GVRZ, Cham, Switzerland

ThP 157 **Analysis of Combustion Byproducts on Firefighter Protection Equipment Using a Novel High Resolution GC/Q-TOF**; Christiane Hoppe-Jones[1]; Sofia Nieto[2]; Nathan Eno[2]; Shane Snyder[1]; [1]University of Arizona, Tucson, AZ; [2]Agilent Technologies, Inc., Santa Clara, CA

ThP 158 **Detection of Novel Perfluorinated Ether Sulfonates in Wildlife in South Carolina and Florida**; Jackie Bangma[1]; Jessica L Reiner[2]; Russell H Lowers[3]; John A. Bowden[2]; [1], Charleston, SC; [2]National Institute of Standards and Technology, NIST, Hollings Marine Laboratory, Charleston, SC; [3]Integrated Mission Support Services, Titusville, FL

ThP 159 **Analysis of Compounds Derived from Aquatic Plastic Pollution by GC-TOFMS**; Kathryn M Renyer[1]; John J Kelly[1]; Timothy J Hoellien[1]; Daryl Giblin[2]; M. Paul Chiarelli[1]; Michael L. Gross[2, 3]; [1]Loyola University, Chicago, IL; [2]Washington University, St Louis, MO; [3]Washington University School of Medicine, St Louis, MO

ThP 160 **Evaluation of a Novel Combination Sampler/ Reagent with Liquid Chromatography Coupled to Tandem Mass Spectrometry Detection to Measure 4,4'-Methylenediphenyldiisocyanate Atmospheres**; Sebastien Gagne[1]; Silvia Puscasu[1]; Simon Aubin[1]; Philippe Sarazin[1]; Mark Spence[2]; [1]IRSST, Montreal, Qc; [2]III, Manchester, UK

ThP 161 **Mass Fragment and Neutral Loss Database for Non-Target Environmental Analysis by Liquid Chromatography/High Resolution Mass Spectrometry**; Shigeru Suzuki[1]; Mari Takazawa[1]; Atsuko Hasegawa[2]; Michiko Uebori[1]; Yasuko Yoshida[3]; Masahiko Takino[4]; Kaori Okubo[5]; Miho Shinomiya[6]; [1]Chubu University, Kasugai, Aichi; [2]Kanagawa Environmental Research Center, Hiratsuka, Japan; [3]Sumica Chemical Analysis Service Ltd., Tokyo, Japan; [4]Agilent Technologies Japan Ltd., Hachioji, Japan; [5]Saga Pharmaceutical Sanitation Center, Saga, Japan; [6]Saitama Prefectural University, Kasukabe, Japan

ThP 162 **Two-Dimensional Liquid Chromatography Coupled with High-Resolution Mass Spectrometry: Application for Analysis of Complex Surfactant Mixtures in Aquatic Environments**; Sarah Choyke[1]; Bernadette Vogler[2]; Gordon Getzinger[1]; P. Lee Ferguson[1]; [1]Duke University, Durham , NC; [2]EAWAG, Dübendorf, ZH

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ThP 164 **Non-Targeted Screening of More than 20 Ethoxylated Homologs and their Transformation Products in Water Samples Using High Resolution-Mass Spectrometry**; Maryam Khaksari[1, 2]; Lynn R Mazzoleni[1, 2]; [1]Chemical Advanced Resolution Methods, Michigan Technological University, Houghton, Michigan; [2]Department of Chemistry, Michigan Technological University, Houghton, MI

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ThP 167 **The Analysis of Environmental Samples Using High Resolution Mass Spectrometry to Identify Novel PFAS Compounds**; Paul C. Winkler[1]; Simon Roberts[1]; Craig Butt[1]; Christopher Borton[1]; [1]SCIEX, Framingham, MA

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ThP 169 **High Resolution Mass Spectrometry Discovery of N-Halogenated-Peptides in Drinking Water**; Ping Jiang[1]; Guang Huang[1]; Lindsay Jmaiff Blackstook[1]; Xing-Fang Li[2]; [1]University of Alberta, Edmonton, Alberta; [2]University of Alberta, Edmonton, AB, Canada

ThP 170 **Qualitative Analysis of Halogenated Organic Compounds Unintentionally Generated in Municipal Waste Water Treatment Plants**; Mari Takazawa[1]; Shigeru Suzuki[1]; Takeshi Nakano[2]; Shinji Tsunoi[2]; Miho Shinomiya[3]; [1]Chubu University, Kasugai, Japan; [2]Osaka University, Research Center for Environmental Preservation, Suita, Japan; [3]Saitama Prefectural University, Kasukabe, Japan

ThP 171 **Structural Elucidation and Differentiation of Azo Disperse Dyes Containing Different Substituents at the Benzene Core**; Nadia Sultana[1]; Nelson R. Vinueza[1]; [1]Department of Textile Engineering, Chemistry and Science, NC State Univeristy, Raleigh, NC

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ThP 173 **Molecular-level Insights into the Increased Toxicity of Crude Oil Environmental Transformation Products**; Phoebe Zito[1]; Huan Chen[1]; Amy M McKenna[1]; David C Podgorski[1, 2]; Steven M. Rowland[1, 3]; Jie Lu[3]; Yuri E Corilo[1, 3]; Ryan P. Rodgers[1]; [1]National High Magnetic Field Laboratory,

Florida State University, Tallahassee, FL; [2]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL; [3]Future Fuels Institute, Florida State University, Tallahassee, FL

ThP 174 **Determination of Per/Polyfluoroalkyl Substances (PFAS) in Water Using HPLC/MS/MS**; Tarun Anumol[1]; Theresa Sosienski[2]; Craig Marvin[1]; Dan-Hui Dorothy Yang[2]; Patrick Jeanville[2]; *[1]Agilent Technologies, Inc., Wilmington, DE; [2]Agilent Technologies, Inc., Santa Clara, CA*

ThP 175 **Determination Nitrosamines in Drinking Water by GC-Triple Quadrupole Mass Spectrometry**; Louis Maljers[1]; Steve Fannin[2]; *[1]Bruker Daltonics, andover, ma; [2]Bruker Daltonics, Billerica, MA*

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ThP 177 **Preferential Cleavage at Lysine Residues Upon Activation of [M-H-NH3]+derived from Ion/Ion Reactions with the Gold Dichloride Reagent Anion.**; David J Foreman[1]; Stella K Betancourt[1]; Scott A McLuckey[1]; *[1]Purdue University, West lafayette, Indiana*

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ThP 179 **Identification of Phospho- and Sulfopeptides via Charge Inversion Ion/Ion Reactions and Dipolar DC Collisional Activation**; Mack Shih[1]; Scott A McLuckey[1]; *[1]Purdue University, West lafayette, Indiana*

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ThP 181 **The Dissociation and Ion Molecule Reaction Pathways of Gas-Phase Complexes Composed of Alkaline Earth Metals Coordinated by Alcohol Ligands**; Sarah Sheffield[1]; Susan Kline[1]; Jordan Pestok[1]; Michael Van Stipdonk[1]; *[1]Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA*

ThP 182 **A Gas-Phase Study of the Nucleophilic Halogenation of Aromatic Heterocycles**; Leah Donham[1]; Scott Gronert[1]; *[1]Virginia Commonwealth University, Richmond, VA*

ThP 183 **Electrospray-Based Photo-Catalytic Screening Method for Studying Electronic Effects on Oxidative Dehydrogenation of N-heterocycle Compounds**; Savithra Jayaraj[1]; Abraham K. Badu-Tawiah[2]; *[1]The Ohio State University, Columbus, OH; [2]The Ohio State University, Columbus, OH*

ThP 184 **Exploring Gas Phase Behavior of Small Cationized Non-Covalent Complexes between Hexose-Phosphate and Basic Compounds Using H/D Exchanges**; Ekaterina Dariy[1, 2, 3]; Yves Gimbert[4]; Sandra Alves[5]; Alain Perret[1, 2, 3]; Jean-Claude Tabet[5, 6]; *[1]Commissariat à l'Energie Atomique et aux Energies Alternatives, Direction de la Recherche Fondamentale, Institut de Génomique, Evry, France; [2]Université d'Evry Val d'Essonne, Evry, France; [3]Centre National de la Recherche Scientifique, UMR8030, Génomique métabolique, Evry, France; [4]Université Grenoble Alpes (DCM), CNRS-UJF 5250, BP 38041, Grenoble, France; [5]Sorbonne Universités, UPMC Univ Paris 06, CNRS, Institut Parisien de Chimie Moléculaire, Paris, France; [6]Commissariat à l'Energie Atomique et aux Energies Alternatives, iBiTec-S, SPI, LEMM, Gif Sur Yvette, France*

ThP 185 **Going Where Few Dare To: Exploring the Intrinsic Reactions of Uranyl-Oxo and -Oxo Hydride Anions with H2O and O**; Michael J. Van Stipdonk[1]; Evan Perez[2]; Cassandra Hanley[1]; Irena Tatosian[1]; Amanda Bubas[1]; *[1]Duquesne University, Pittsburgh, PA; [2]Yale University, New Haven, CT*

ThP 186 **Flame Atmospheric Pressure Chemical Ionization Coupled with Negative Electrospray Ionization Mass Spectrometry for Ion Molecule Reactions**; Sy-Chyi Cheng[1]; Suhail Muzaffar Bhat[1]; Jentaie Shiea [1]; *[1]National Sun Yat-Sen University, Kaohsiung, Taiwan*

ThP 187 **Manipulation of conformation via charge and temperature. An ion mobility mass spectrometry investigation**; Jacquelyn R Jhingree[1]; Jakub Ujma[2]; Perdita E Barran[1]; *[1]University of Manchester, Manchester, UK; [2]Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK*

ThP 188 **A FT-3D Ion Trap with In-Trap Electron Ionization and Pulsed Gas Inlet: Transient Pressure Profile and Space Charge Induced Effects**; Yessica Brachthaeuser[1]; David Mueller[1]; Hendrik Kersten[1]; Klaus J. Brockmann[1]; Valerie Derpmann[2]; Michel Aliman[2]; Thorsten Benter[1]; *[1]Bergische Universität Wuppertal, Wuppertal, NRW; [2]Zeiss SMT GmbH, Oberkochen, Germany*

ThP 189 **Ion Dynamics Simulation: Space Charge Effects in a Fourier Transform 3D-Ion Trap (FT-ion trap)**; Walter Wissdorf[1]; Christine Polaczek[1]; Yessica Brachthäuser[1]; Hendrik Kersten[1]; Albrecht Brockhaus[1]; Michel Aliman[2]; Valerie Derpmann[2]; Alexander Laue[2]; Thorsten Benter[1]; *[1]Bergische Universität Wuppertal, Wuppertal, NRW; [2]Zeiss SMT GmbH, Oberkochen, Germany*

ThP 190 **Systematic Studies of the Impact of Chemical Modifiers on the Ion Population Observed with Nano Electrospray Ionization (nESI) Mass Spectrometry**; Marco Thinius[1]; Christine Polaczek[1]; Clara Markert[1]; Duygu Erdogdu[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]Bergische Universität Wuppertal, Wuppertal, NRW*

ThP 191 **Fast Space Charge Simulations: Simulation of Ion – Ion and Background Gas Interaction in a Linear Quadrupole**; Walter Wissdorf[1]; Hendrik Kersten[1]; Thorsten Benter[1]; Tom Covey[2]; Jim Hager[2]; Bradley B Schneider[2]; *[1]Bergische Universität Wuppertal, Wuppertal, NRW; [2]SCIEX, Concord, ON, Canada*

ThP 192 **Effects of Chemical Dynamics and Clustering Reactions of Chemical Modifiers with Analyte Ions in Differential Mobility Spectrometry (DMS)**; Florian Stappert[1]; Marco Thinius[1]; Hendrik Kersten[1]; Walter Wissdorf[1]; Tom Covey[2]; Bradley B Schneider[2]; Jim Hager[2]; Thorsten Benter[1]; *[1]Bergische Universität Wuppertal, Wuppertal, NRW; [2]SCIEX, Concord, ON, Canada*

ThP 193 **Characterization of Unusual CO2 and N2 Adducts to Gas-phase Copper Ion using Isotope Labeling and High-accuracy Mass Measurements**; Luke Metzler[1]; Stephen Koehler[1]; Arpad Somogyi[2]; Michael J. Van Stipdonk[1]; *[1]Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA; [2]Mass Spectrometry and Proteomics Facility, Campus Chemical Instrument Center, Columbus, OH*

ThP 194 **Reactivity of Amino Acid Anions with Atomic Species in the Interstellar Medium**; Zhechen Wang[1]; Veronica M. Bierbaum[1]; Yake Li[1]; *[1]University of Colorado at Boulder, Boulder, CO*

ThP 195 **Creation and Intrinsic Reactions of Gas-phase Group II Cation-carbanion Complexes**; Stephen Koehler[1]; Cassandra Hanley[1]; Nevo Polonsky[1, 2]; Jordan Pestok[1];

Michael J. Van Stipdonk[1]; [1]*Duquesne University, Pittsburgh, PA;* [2]*Bates College, Lewiston, ME*

ThP 196 **Gas-phase Rearrangement Reaction of Schiff-Base-Modified Peptide Ions**; Nan Wang[1]; Alice L Pilo[2]; Jiexun Bu[1]; Scott A McLuckey[1]; [1]*Purdue University, West Lafayette, IN;* [2]*Merck & Co., Inc, Rahway, NJ*

ThP 197 **Oxygen Peribridged Quinolinium Biradicals: Gas-Phase Reactivity Study by Using a Linear Quadrupole Ion Trap (LQIT) Mass Spectrometer**; Raghavendhar R Kotha[1]; Ravikiran Yerabolu[1]; John J Nash[1]; Hilkka I Kenttamaa[1]; [1]*Purdue University, West lafayette, Indiana*

ThP 198 **Identification of Glucuronidation Sites in Protonated Drug Metabolites by Using Ion-Molecule Reactions and Energy-Resolved Mass Spectrometry**; Edouard Niyonsaba[1]; Xin Ma[1]; Zaikuan Yu[1]; John Kong[1]; Hilkka Kenttämaa[1]; [1]*Purdue University, West Lafayette, IN*

ThP 199 **5-Dehydroquinoline Radical Cation: a New Reactive σ,σ-Biradical Formed via Isomerization from 5-Iodo-8-Dehydroquinolinium Cation**; Xin Ma[1]; Chunfen Jin[1]; John J. Nash[1]; Hilkka I. Kenttämaa[1]; [1]*Purdue University-Department of Chemistry, West Lafayette, IN*

ThP 200 **Gas-Phase Synthesis and Reactivity of Diphenylphosphonium Cations**; Xinchi Yin[1]; Yuanjiang Pan[1]; [1]*Department of Chemistry, Zhejiang University, Hangzhou, China*

ThP 201 **The tautomerism of Phosphonium Cations in the Gas Phase**; Xinchi Yin[1]; Shanshan Shen[1]; Yuanjiang Pan[1]; [1]*Department of Chemistry, Zhejiang University, Hangzhou, China*

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ThP 203 **Tracking Conformational Dynamics and Ligand Binding in Membrane Proteins Using HDX-MS**; Martin Lorenz Eisinger[1]; Layin Nie[1,2]; Aline Ricarda Doerrbaum[1,3]; Hartmut Michel[1]; Etana Padan[4]; Julian Langer[1,3]; [1]*MPI for Biophysics, Frankfurt am Main, Hessen;* [2]*University of Oxford, Oxford, UK;* [3]*MPI for Brain Research, Frankfurt am Main, Germany;* [4]*Hebrew University, Jerusalem, Israel*

ThP 204 **Sequential Conformational Changes in Influenza Hemagglutinin during Fusion Activation**; Mark Benhaim; *University of Washington, Seattle, WA*

ThP 205 **Investigation of Interactions between Beta-Lactamases and Beta-Lactamase Inhibitory Protein(BLIP) Using Hydrogen/Deuterium Exchange Mass Spectrometry(HDX-MS)**; Liwen Huang[1]; Pui-kin So[1]; Yun-chung Leung[1]; Zhong-ping Yao[1]; [1]*The Hong Kong Polytechnic University, Hong Kong, China*

ThP 206 **HDX MS of the Largest Soluble Human Glycoprotein, Von Willebrand Factor**; Roxana E. Iacob[1]; Klaus Bonazza[2]; Timothy A. Springer[3]; John R. Engen[4]; [1]*Northeastern University , Boston, MA;* [2]*Children's Hospital Boston and Harvard Medical School, Boston, MA;* [3]*Children's Hospital Boston and Harvard Medical School, Boston, MA;* [4]*Northeastern University, Boston, MA*

ThP 207 **Use of Differential Hydrogen/Deuterium Exchange Mass Spectrometry to Support Ligand Binding Mode Predictions within the Vitamin D Receptor**; Ryan Stites[1]; Scott Novick[2]; Bruce D Pascal[2]; Quanrong Shen[1]; Michael J Chalmers[1]; Patrick R Griffin[2]; Jeffrey A Dodge[1]; [1]*Eli Lilly and Company, Indianapolis, IN;* [2]*The Scripps Research Institute, Jupiter, FL*

ThP 208 **Hydrogen Deuterium Exchange Mass Spectrometry of RORgt Modulators Show Conformational Changes and Allosteric Binding Site**; Rebecca Rae[1]; Yafeng Xue[2]; Anna Aagaard[2]; Frank Narjes[3]; [1]*Department of Medicinal Chemistry, Respiratory, Inflammation & Autoimmunity, Innovative Medicines and Early Development Biotech Unit, AstraZeneca, Gothenburg, Sweden;* [2]*Discovery Sciences, AstraZeneca, Gothenburg, Sweden;* [3]*Department of Medicinal Chemistry, Respiratory, Inflammation & Autoimmunity, Innovative Medicines and Early Development Biotech Unit, Gothenburg, Sweden*

ThP 209 **Using Hydrogen/Deuterium Exchange-Mass Spectrometry to Probe Changes in Enzyme Dynamics during Catalysis**; Courtney S Fast[1]; Siavash Vahidi[1]; Lars Konermann[1]; [1]*University of Western Ontario, London , ON, Canada*

ThP 210 **Conformational Changes in Active/Inactive States of PP2Cα Characterized byHydrogen-Deuterium Exchange Mass Spectrometry**; Kyle W Anderson[1,2]; Sharlyn J Mazur[3]; Subrata Debnath[3]; Elyssia S Gallagher[1,2]; Stewart R Durell[3]; Ettore Appella[3]; Jeffrey W Hudgens[1,2]; [1]*National Institute of Standards and Technology, Gaithersburg, MD;* [2]*IBBR, Rockville, MD;* [3]*National Cancer Institute, Bethesda, MD*

ThP 211 **Development of a Hydrogen Exchange-Mass Spectrometry Method to Predict Aggregation Propensity of Protein Therapeutics**; Juan P Rincon[1]; Gulsum Meric[2]; Cesar Calero-Rubio[2]; Christopher O'Brien[2]; Anne Robinson[3]; Christopher J Roberts[2]; David D Weis[1]; [1]*University of Kansas, Lawrence, Kansas;* [2]*University of Delaware, Newark, Delaware;* [3]*Tulane University, New Orleans, Louisiana*

ThP 212 **HDX-MS Reveals a Common Binding Surface for Endogenous Peptide- and Protein Ligands to the Sortilin Receptor**; Esben Trabjerg[1,2]; Fredrik Kartberg[2]; Søren Christensen[2]; Kasper D Rand[1]; [1]*Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark;* [2]*Department of Biologics, H. Lundbeck A/S, Valby, Denmark*

ThP 213 **Pulsed HDX Illuminates the Aggregation Kinetics of Alpha Synuclein, the Causative Agent for Parkinson's Disease**; Eva T. Illes-Toth[1]; Don L. Rempel[1]; Michael L. Gross[1]; [1]*Washington University in St Louis, St. Louis, MO*

ThP 214 **Discovery and Structural Analysis of Selective Modulators for Retinoic-Acid Receptor-Related Orphan Receptor RORβ**; Venkat Dharmarajan[1]; Chrsitelle Doebelin[1]; Ted Kamenecka[1]; Ruben Garcia-Ordonez[1]; Patrick R Griffin[1]; [1]*The Scripps Research Institute, Jupiter, FL*

ThP 215 **Hydrogen Deuterium Exchange of Native Ubiquitin Probed by hv-ECD with Complete Sequence Coverage**; Yury V. Vasil'ev[1]; Nathan I. Lopez[1]; Valery G. Voinov[2]; Joseph S. Beckman[1]; [1]*Linus Pauling Institute, Oregon State University, Corvallis, OR;* [2]*e-MSion, Corvallis, OR*

ThP 216 **Mapping Substrate Binding Sites of Low Affinity Ligands to a Glycosyltransferase Using HDXMS**; Deepa Balasubramaniam[1]; Thierry Fischmann[1]; Todd Mayhood[1]; Michael Kavana[2]; George Addona[2]; Maria Webb[1]; Payal Sheth[1]; David McLaren[1]; [1]*Merck, Kenilworth , NJ;* [2]*Merck & Co., Inc., Boston, MA*

ThP 217 **Effects of N and C Terminal Truncations on Heme Oxygenase 2 Examined via Hydrogen Deuterium Exchange Mass Spectrometery**; Brent A. Kochert[1]; Angela S. Fleischhacker[2]; Stephen W. Ragsdale[2]; John R. Engen[1]; [1]*Northeastern University, Boston, MA;* [2]*University of Michigan, Ann Arbor, Michigan*

ThP 218 **HDX-MS and Molecular Dynamics Simulations Provide Complementary Insights Into The Mechanisms of Allosteric Protein Regulation**; Yiming Xiao[1]; Gary S Shaw[2]; Lars Konermann[2]; [1]*University of Western Ontario,*

London, ON, Canada; [2]University of Western Ontario, London , ON, Canada

ThP 219 **Dissection of Key Conformational Changes in the Regulatory Domains of BTK upon Lipid Interaction: is the Full-Length Kinase Necessary?**; Charles Mundorff[1]; Thomas E. Wales[1]; Raji E. Joseph[2]; Amy H. Andreotti[2]; John R. Engen[1]; *[1]Northeastern University, Boston, MA; [2]Iowa State University, Ames, IA*

ThP 220 **Characterizing the Binding Interface between Human Insulin-like Growth Factor and its Binding Protein by Hydrogen/Deuterium Exchange Mass Spectrometry**; Paul A. Salinas[1]; Hanwei Zhao[1]; Justin M. Prien[1]; Bernice Yeung[1]; *[1]Shire HGT, Lexington, MA*

ThP 221 **HDX-MS and Quantitative Crosslinking-MS (XL-MS) Reveals NR AF2 Dynamics Controlling Receptor Activity and Target Gene Promoter Specificity**; Jie Zheng[1]; Bruce D. Pascal[1]; Ruben Garcia-Ordonez[1]; Scott Novick[1]; Mira Chang[1]; Patrick R Griffin[1]; *[1]The Scripps Research Institute, Jupiter, FL*

ThP 222 **Implementation of HDX-MS and SCA to Elucidate the Role of Allosteric Coupling during Electron Transport in Transhydrogenase Complexes**; Luke Berry[1]; Saroj Poudel[1]; Monika Tokmina-Lukaszewska[1]; Dan Coleman[1]; Gerrit J. Schut[2]; Michael W.W. Adams[2]; John Peters[3]; Eric Boyd[1]; Brian Bothner[1]; *[1]Montana State University, Bozeman, MT; [2]University of Georgia, Athens, GA; [3]Washington State University, Pullman, WA*

ThP 223 **Allosteric Conformational Change of KEAP1 upon Nrf2 Binding Based on Hydrogen/Deuterium Exchange Monitored by 21 T FT-ICR Mass Spectrometry** ; Peilu Liu[1, 2]; Mengqi Zhong[3]; Adrian Whitty[3]; Alan G. Marshall[1, 2]; *[1]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL; [2]National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; [3]Department of Chemistry, Boston University, Boston, MA*

ThP 224 **Application of Hydrogen-Deuterium Exchange Mass Spectrometry to Interrogate the Dynamic Conformational Regulation of BCL-2 Family Proteins**; Susan Lee[1]; Lauren A Barclay[1]; Thomas E Wales[2]; Franziska Wachter[1]; Gregory H Bird[1]; John R Engen[2]; Loren D Walensky[1]; *[1]Dana Farber Cancer Institute, Boston, MA; [2]Northeastern University , Boston, MA*

ThP 225 **Probing Mutations in the Tec-Family Tyrosine Kinase BTK Using NMR, HXMS, and a Combined Domain Building Block Approach**; Thomas E. Wales[1]; Raji E. Joseph[2]; Amy H. Andreotti[2]; John R. Engen[3]; *[1]Northeastern University, Boston, MA; [2]Iowa State University, Ames, IA; [3]Northeastern University, Boston, MA*

ThP 226 **Fishing for Calmodulin via a Disordered Bait of the Adenylate Cyclase Toxin**; Darragh P. O'Brien[1]; Dominique Durand[2]; Véronique Hourdel[1]; Maryline Davi[1]; Julia Chamot-Rooke[1]; Patrice Vachette[2]; Sébastien Brier[1]; Daniel Ladant[1]; Alexandre Chenal[1]; *[1]Institut Pasteur, Paris, France; [2]Université Paris-Sud 11, Paris, France*

ThP 227 **Epitope Mapping of Malaria Antigens by HDX-MS: DBP and CelTOS from *Plasmodium vivax* and *Plasmodium falciparum***; Yining Huang[1]; Ben Niu[1]; Jagat Adhikari[1]; Nicole Salinas[2]; Darya Urusova[3]; Niraj Tolia[3]; Michael L. Gross[1]; *[1]Washington University in St Louis, St. Louis, MO; [2]Washington University School of Medicine, St Louis, MO; [3]Washington University School of Medicine, St. Louis, MO*

ThP 228 **Stress Dependent Dimerization of Monoclonal Antibody Probed by Hydrogen Deuterium Exchange Mass Spectrometry**; Devrishi Goswami[1]; Jun Zhang[1]; Christopher Pierini[1]; *[1]Amgen Inc., Thousand Oaks, CA*

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ThP 229 **Uniformly 13C Labelled Compounds from Arthrospira as Multiple Internal Standards for Quantitative Isotope-Dilution Mass Spectrometry of 74 Key Bacterial Metabolites**; Salah Abdelrazig[1]; Sarah Schatschneider[2]; Laudina Safo[1]; Anne M. Henstra[3]; Thomas Millat[3]; Dong-Hyun Kim[1]; Klaus Winzer[3]; Nigel Minton[3]; David A. Barrett[1]; *[1]Centre for Analytical Bioscience, School of Pharmacy, University of Nottingham, Nottingham, UK; [2]Evonik Nutrition & Care, Halle-Westfalen, Germany; [3]Synthetic Biology Research Centre, University of Nottingham, Nottingham, UK*

ThP 230 **Characterization of Organic Light Emitting Diode Materials via High Resolution Liquid Chromatography Mass Spectrometry**; Kyuhyun Im; *Samsung, Suwon*

ThP 231 **Phased Spectrum Decomposition Method – A Super-Resolution Algorithm for Fourier Transform Mass Spectrometry**; Konstantin Aizikov[1]; Dmitry Grinfeld[1]; Arne Kreutzman[1]; Eugen Damoc[1]; Oliver Lange[1]; Alexander Makarov[1]; *[1]Thermofisher, Bremen, Bremen*

ThP 232 **Enhanced Mass Accuracy in Multi-Reflecting TOF MS**; Boris Kozlov[1]; Richard Denny[1]; Yuriy Khasin[2]; Sergey Kirillov[2]; Vasiliy Makarov[2]; Anatoly Verenchikov[2]; John Hoyes[1]; *[1]Waters Corporation, Wilmslow, UK; [2]MS Consulting, Bar, Montenegro*

ThP 233 **An Innovative Algorithm to Elucidate the Structure of Unknown Compounds Using Tandem Mass Spectrometry and NMR Data**; Elisabeth Ortega-Carrasco[1]; Tatiana Radchenko[1, 2]; Guillem Plasencia[1]; Ismael Zamora[1, 3]; *[1]Lead Molecular Design, S.L., Sant Cugat del Valles, Spain; [2]Universitat Pompeu Fabra, Barcelona, Spain; [3]Molecular Discovery, London, UK*

ThP 234 **Development and Validation of an UHPLC-MS/MS Analytical Method for Trace-Level Detection and Quantitation of Potential Endocrine Disrupting Phytoestrogens in Estuaries**; Jingyi Qi[1]; Vanisree Mulabagal[1]; Lan Liu[1]; Joel S Hayworth[1]; *[1]Auburn University, Auburn, AL*

ThP 235 **Prediction of Mass Resolving Power of Linear TOF Involving Sample Thickness by Time-Domain Analysis**; Yi-Hong Cai[1]; Yi-Sheng Wang[1]; *[1]Genomics Research Center Academia Sinica, Taipei*

ThP 236 **Origin Discrimination of Carrots Using UHPLC-Q-Orbitrap HRMS with Multivariate Analysis**; Dongjin Kang[1]; Ji-Yong Moon[1]; Seong-Hun Lee[1]; *[1]National agricultural products quality management service, Gimcheon-si, Gyeongsangbuk-do*

ThP 237 **Revolutionary Proteome Profiling and Quantitation without Compromising Speed, Sensitivity, and Selectivity**; Yue Xuan[1]; Oleksandr Boychenko[2]; Remco Swart[2]; Alexander Harder[1]; Thomas Moehring[1]; *[1]Thermo Fisher Scientific, Bremen, Germany; [2]Thermo Fisher Scientific, Germering, Germany*

ThP 238 **Utilizing High Resolution Accurate Mass for the Quantitation of Therapeutic Peptides in Human Plasma**; Keeley Murphy [1]; Jonathan Josephs[2]; David Brant[2]; *[1]Thermo Fisher Scientific, San Jose , CA; [2]ThermoFisher, San Jose, CA*

ThP 239 **Advanced Data Visualization: The Many Dimensions of Petroleomics using High-Resolution Gas Chromatography and Time-of-Flight Mass Spectrometry**; Christina Kelly[1]; Jonathan D Byer[1]; Joe Binkley[1]; Lorne Fell[1]; *[1]LECO Corporation, Saint Joseph, MI*

ThP 240 **Identification of Novel Opioid Interferences Using High-Resolution Accurate Mass Spectrometry**; Ana Celia Grenier[1]; Teresa M Pekol[1]; Dana L Schubring[1]; Charlene Johnson[1]; Lawrence J. Andrade[1]; *[1]Dominion Diagnostics, North Kingstown, RI*

ThP 241 **Quantitative Determination of Protein-Ligand Affinity by Online SEC High-Resolution Native Mass Spectrometry**; Chengfeng Ren[1]; Aaron Bailey[2]; Erica VanderPorten[1]; Angela Oh[1]; Wilson Phung[1]; Seth A. Harris[1]; Yichin Liu[1]; Wendy Sandoval[1]; Guanghui Han[1]; *[1]Genentech, Inc, South San Francisco, CA; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 242 **A New Release of the NIST Mass Spectrum Analyzer MS Interpreter to the Work with Fractional Mass Spectrums**; Alexey Mayorov[1, 2]; Stephen E Stein[3]; Dmitrii V. Tchekhovskoi[3]; Yuri Mirokhin[3]; *[1]NIST, Gaithersburg, MD; [2]Emanuel Institute of Biochemical Physics of Russian Academy of Sciences, Moscow, Russia; [3]NIST, Gaithersburg, MD*

ThP 243 **Efficient Identification of Complete Unknowns Using Isotope Modeling and High Resolution, Accurate Mass Data**; Jonathan Marshall[1]; Michael Peddicord[1]; *[1]Bristol-Myers Squibb, New Brunswick, NJ*

ThP 244 **High Mass Accuracy/Resolution Mass Spectrometry in Sensitive Analysis of Tropane Alkaloids**; Kui Yang[1]; Michael Hadwiger[1]; Michael Trehy[1]; David A. Keire[1]; *[1]Division of Pharmaceutical Analysis, Office of Testing and Research, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, St. Louis, MO*

ThP 245 **Fast Algorithms for Comparing and Clustering Tandem Mass Spectra**; Lei Wang[1]; SUJUN LI[1]; Haixu Tang[1]; *[1]Indiana University Bloomington, Bloomington, IN*

ThP 246 **Using SWATH Acquisition with Differential Ion Mobility for Accurate Mass Flux Analysis**; Tiago Cardoso Alves[1]; Keith J. Goodman[2]; Sabu George[3]; Abhishek Jha[3]; Rebecca L. Cardone[4]; Richard G. Kibbey[4]; *[1]Yale University, New Haven, CT; [2]SCIEX, Framingham, MA; [3]Elucidata, Cambridge, MA; [4]Yale University, New Haven, CT*

ThP 247 **Leveraging Targeted and Untargeted FTMS Applications via Advanced Processing of Transients and Big Data Analysis**; Konstantin O. Nagornov[1]; Anton N. Kozhinov[1]; Andrey A. Laktionov[1]; Yury O. Tsybin[1]; *[1]Spectroswiss Sàrl, Lausanne, Switzerland*

ThP 248 **Monitoring Critical Quality Attributes of mAbs at Subunit and Peptide Level Using a Single High Resolution LCMS Platform**; Jing Fang[1]; Nilini Ranbaduge[1]; Henry Shion[1]; Min Du[1]; Ying Qing Yu[1]; Scott Berger[1]; Weibin Chen[1]; *[1]Waters Corp, Milford, MA*

ThP 249 **Unprecedented Isobaric Complexity in Long Range Transported Atmospheric Aerosol Observed Using Fourier Transform Ion Cyclotron Resonance Mass Spectrometry**; Simeon K Schum[1]; Lynn R Mazzoleni[1]; *[1]Michigan Technological University, Houghton, MI*

ThP 250 **Performance Metrics and Example Applications:Orbitrap Mass Spectrometry at Resolving Power 1M**; Jesse D. Canterbury[1]; Seema Sharma[2]; Tim J. Stratton[2]; Mike Senko[3]; Vlad Zabrouskov[2]; Eduard Denisov[4]; Alexander Makarov[4]; *[1]Thermo Scientific, San Jose, CA; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, San Jose, California; [4]Thermo Fisher Scientific, Bremen, Germany*

ThP 251 **Quantitative Bidimensional (2D) Fourier Transform Mass Spectrometry**; Julien Bouclon[1]; Fabrice Bray[2]; Geoffrey Bodenhausen[1]; Christian Rolando[2]; *[1]Laboratoire des Biomolécules, Ecole Normale Supérieure, Paris, France; [2]MSAP, Université de Lille 1, Villeneuve d'ASCQ, France*

ThP 252 **Automatization of Workflow for Complex Mixture Analysis**; Vlad Lobodin; *MAXIKAT, INC., Tallahassee, FL*

ThP 253 **Ion Current-based Proteomic Profiling of Mitoxantrone and KX02 Treatment in Mouse Glioma 261 Cells Reveals Elevated Innate Immune Response**; Chengjian Tu[1]; Yahao Bu[2]; Jun Li[1]; James Clements[2]; David Hangauer[2]; Jun Qu[1]; *[1]University at Buffalo, Buffalo, NY; [2]Athenex Pharmaceuticals LLC, Buffalo, NY*

ThP 254 **Monitoring Critical Quality Attributes Supporting Development of Biopharmaceuticals**; Sean McCarthy[1]; Sibylle Heidelberger[2]; *[1]SCIEX, Framingham, MA; [2]SCIEX, Concord, ON, Canada*

ThP 255 **Mass Accuracy and Robustness of Intact mAb on the X500B Benchtop Quadrupole-Time-Of-Flight Instrument**; Fan Zhang[1]; Chris Nortcliffe[2]; Sibylle Heidelberger[3]; *[1]SCIEX, Redwood City, CA; [2]Sciex, Warrington, UK; [3]SCIEX, Concord, ON, Canada*

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ThP 257 **ToF-SIMS Investigations of Tip-Surface Chemical Interactions in Atomic Force Microscopy on a Combined AFM/ToF-SIMS Platform**; Chance C. Brown[1, 2]; Anton V. Ievlev[1]; Petro Maksymovych[1]; Sergei V. Kalinin[1]; Olga S. Ovchinnikova[1]; *[1]Oak Ridge National Lab, Oak Ridge, TN; [2]University of Tennessee, Knoxville, TN*

ThP 258 **Bioimaging *via* LA-ICP-MS - a Powerful Analytical Tool for the Investigation of the Anti-Cancer Drug Cisplatin**; Oliver Bolle Bauer[1]; Christina Köppen[1]; Giuliano Ciarimboli[2]; Hans-Joachim Schurek[2]; Michael Sperling[1]; Uwe Karst[1]; *[1]Institute of Inorganic and Analytical Chemistry, University of Muenster, Muenster, Germany; [2]University Hospital of Münster, Department of Experimental Nephrology, Muenster, Germany*

ThP 259 **Laser Ablation-halo-Flowing Atmospheric Pressure Afterglow-Mass Spectrometry: Method Development and Applications**; Valérie Brueckel[1]; Michael Sperling[2]; Jacob Shelley[3]; Uwe Karst[1]; *[1]University of Muenster, Institute of Inorganic and Analytical Chemistry, Muenster, Germany; [2]European Virtual Institute for Speciation Analysis, Muenster, Germany; [3]Rensselaer Polytechnic Institute, Department of Chemistry and Chemical Biology, Troy, NY*

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ThP 332 **Deep Learning for Peptide Identification**; Wout Bittremieux[1]; Kris Laukens[1]; *[1]University of Antwerp, Antwerp*

ThP 333 **Functional 5' UTR Motif Discovery with LESMoN: Local Enrichment of Sequence Motifs in Protein-Protein Interaction Networks**; Mathieu Lavallée-Adam[1, 2]; Philippe Cloutier[3]; Benoit Coulombe[3, 4]; Mathieu Blanchette[2]; *[1]University of Ottawa, Ottawa, ON, Canada; [2]McGill University, Montréal, Quebec; [3]Institut de recherches cliniques de Montréal, Montreal, QC, Canada; [4]Université de Montréal, Montréal, QC, Canada*

ThP 334 **The Database for Mining Biomarkers in the Brain Tumor Tissue Mass-Spectra**; Anatoly Sorokin[1]; Vsevolod Shurhkhay[2]; Igor Popov[1]; Evgeny Zhvansky[1]; Nikita Levin[1]; Alexander Potapov[2]; Eugene (Evgeny) Nikolaev[1, 3, 4]; *[1]Moscow Institute of Physics and Technology (State University), Dolgoprudnyj, Russia; [2]N. N. Burdenko Scientific Research Neurosurgery Institute, Moscow, Russia; [3]Skolkovo institute of science and technology, Skolkovo, Russia; [4]Institute of energy problems of chemical physics Russian Academy of Sciences, Moscow, Russia*

ThP 335 **Bayesian Identification of Post-Translational Modifications in Isobarically Labeled Mass Spectrometry Data**; Stephen Coleman; *University of Colorado, Boulder, CO*

ThP 336 **New Peak Finding and Integration Algorithms in Skyline**; Nicholas Shulman[1]; Max Horowitz-Gelb[1]; Andreas F Tillack[2]; Michael H Gelb[2]; Bruce H Robinson[2]; Brendan MacLean[1]; *[1]University of Washington Genome Sciences, Seattle, WA; [2]Department of Chemistry, University of Washington, Seattle, WA*

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ThP 337 **MilkyWay: A Galaxy Platform for Quantitative Comparative Analysis of Bottom-Up Proteomic Mass Spectrometry Datasets**; William D Barshop[1]; Hee Jong Kim[1]; James Akira Wohlschlegel[1]; *[1]University of California Los Angeles, Los Angeles, CA*

ThP 338 **pClean: A Powerful Filtration to Remove the Uninformative Signals in MS Spectra for Peptide Identification**; Yamei Deng[1, 2]; Bo Wen[2]; Shaoxing Xu[2]; Lin Wu[1]; Yan Ren[2]; Siqi Liu[2]; *[1]Beijing Institute of Genomics, Chinese Academy of Sciences, Beijing, China; [2]BGI-Shenzhen, Shenzhen, China*

ThP 339 **ProSight Annotator: Freeware for the Generation of UniProt Formatted XML Files Containing Custom User-Specified Features**; Joseph B Greer[1]; Ryan T. Fellers[1]; Richard D. LeDuc[1]; Bryan P. Early[1]; Alexandra J. VanNispen[1]; Paul M. Thomas[1]; Neil L. Kelleher[1]; *[1]Northwestern University, Evanston, IL*

ThP 340 **Analytica: Software for LC-MS Omics Data Analysis and Visualisation**; Simon Perkins[1]; Dean Hammond[1]; Johannes PC Vissers[2]; James I Langridge[2]; Andrew R Jones[1]; *[1]University of Liverpool, Liverpool, Merseyside; [2]Waters Corporation, Wilmslow, UK*

ThP 341 **A Pipeline for the Semi-Automated Processing of Chromatography-Mass Spectrometry Data**; Sonia Liggi[1]; Christine Hinz[1]; Julia Denes[1]; Maria Laura Santoru[2]; Antonio Murgia[1, 2]; Ke-Di Liu[1]; John Fjeldsted[3]; Luigi Atzori[2]; Jules Leether Griffin[1]; *[1]University of Cambridge, Cambridge, UK; [2]Università degli Studi di Cagliari, Cagliari, Italy; [3]Agilent Technologies, Santa Clara, CA*

ThP 342 **Exploring Multiple Independent Variables Associated with Large Proteomics and Metabolomics Datasets Using a Flexible Hierarchical Organization scheme**; Phillip Seitzer[1]; Seth Just[1]; Susan Ludwigsen[1]; Jacob Lippincott[1]; Caleb Emmons[1]; Nick Vincent-Maloney[1]; Jimar Miller[1]; Brian Searle[1, 2]; *[1]Proteome Software, Portland, OR; [2]University of Washington, Seattle, WA*

ThP 343 **Towards the Smart Lab: A Comprehensive Approach to Mass Spectrometry Quality Control**; Wout Bittremieux[1]; Dirk Valkenborg[2]; Kris Laukens[1]; *[1]University of Antwerp, Antwerp; [2]Hasselt University, Diepenbeek, Limburg*

ThP 344 **A Systematic Workflow for Quality Control of MS-Based Proteomics Using a Complex Biological Standard**; Hossein Fazelinia[1]; Hua Ding[1]; Lynn A. Spruce[1]; Steven H. Seeholzer[1]; *[1]Children's Hospital of Philadelphia, Philadelphia, PA*

ThP 345 **Monitoring Data Quality and Managing Project Sample Queues Across Multiple Instruments**; Brett Larsen[1]; James D R Knight[1]; Guomin Liu[1]; Jianping Zhang[1]; Joshua Sandor[1]; Meghan McFadden[1]; Karen Colwill[1]; Anne-Claude Gingras[1, 2]; *[1]LTRI, TORONTO, ON, Canada; [2]Department of Molecular Genetics, University of Toronto, Toronto, ON, Canada*

ThP 346 **MassIVE Data to Knowledge: Large-Scale Reanalysis of Terabytes of Public Human Datasets**; Jeremy Carver[1]; Mingxun Wang[2]; Nuno Bandeira[2]; *[1]UCSD, La Jolla, CA; [2]UCSD, La Jolla, CA*

ThP 347 **Creation and Analysis of an In-house Designer Library for Fecal MS-based Metabolomics**; Johana Revel[1, 2, 3]; Phillip Seitzer[4]; Liping Yang[3]; Adrian Gombart[2, 5]; Jan F. Stevens[2, 3, 6]; Claudia S. Maier[1, 2, 3]; *[1]Department of Chemistry, Oregon State University, Corvallis, OR; [2]Linus Pauling Institute, Oregon State University, Corvallis, OR; [3]Mass Spectrometry Center, Oregon State University, Corvallis, OR; [4]Proteome Software, Portland, OR; [5]Department of Biochemistry and Biophysics, Oregon State University, Corvallis, OR; [6]Department of Pharmaceutical Sciences, Oregon State University, Corvallis, OR*

ThP 348 **Fast Automated Data Backup and System Suitability Processing for Protein Characterization LC-MS Experiments**; Benjamin Nathan Moore; *Genentech, South San Francisco, CA*

ThP 349 **GiaPronto: A One-Click Online Data Analysis and Visualization for Proteomics**; Amber K. Weiner[1, 2, 3]; Simone Sidoli[1]; Sharon J. Diskin[2, 3]; Benjamin A. Garcia[1, 3]; *[1]Epigenetics Institute, University of Pennsylvania Perelman School of Medicine, Philadelphia, PA; [2]Division of Oncology, Department of Pediatrics, Children's Hospital of Philadelphia, Philadelphia, PA; [3]Genomics and Computational Biology, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA*

ThP 350 **MassBank of North America: An Open Access Metadata-Centric, Auto-Curating Repository for Mass Spectra from Different Instrument Platforms**; Gert Wohlgemuth[1]; Sajjan S. Mehta[2]; Oliver Fiehn[1]; *[1]UC Davis, Davis, CA; [2]University of California, Davis, Davis, CA*

ThP 351 **QCloud: Comprehensive Cloud-Based QC system in the Proteomics Laboratory**; Cristina Chiva[1, 2]; Roger Olivella[1, 2]; Eva Borràs[1, 2]; Guadalupe Espadas[1, 2]; Olga Pastor[1, 2]; Amanda Solé[1, 2]; Eduard Sabidó[1, 2]; *[1]Proteomics Unit, Centre de Regulació Genòmica (CRG), Barcelona Institute of Science and Technology (BIST), Dr. Aiguader 88, Barcelona, Spain; [2]Universitat Pompeu Fabra (UPF), Dr. Aiguader 88, Barcelona, Spain*

ThP 352 **A Complete Data Integrity Solution for Quality Control Laboratories using Mass Spectrometry**; Hua Dong[1]; Leo Wang[1]; Loren Smith[1]; *[1]Agilent Technologies Inc., Santa Clara, CA*

INSTRUMENTATION: NEW DEVELOPMENTS IN ION DETECTION
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ThP 353 **Detection of High Mass MADLI Ions with a Charge Detection Rectilinear Ion Trap Mass Spectrometer (CD-RITMS) by Dipolar Resonant Excitation**; Avinash Adhikrao Patil[1]; Chen-Wei Lee[1]; Szu-Wei Chou[1]; Wen-Ping Peng[1]; *[1]National Dong Hwa University, Shoufeng, Taiwan*

ThP 354 **Analytical Application of a Ultrahigh Speed Multichannel Photodiode for a Quadrupole Mass Spectrometer**; Tsung-Chi Chen[1]; Eric C. Hemenway[1]; Hans Schweingruber[1]; Rexford T. Heller[1]; Raman Mathur[1]; Frederick M. Hudson[1]; Eric Huang[1]; Mark Wadsworth[2]; Judd Jenne[2]; Bruce E. Pirger[2]; Eric Howard[3]; Suraj Bhaskaran[2]; Michael Ugarov[1]; Jae C. Schwartz[1]; Alan E. Schoen[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Liverpool, NY; [3]Opsci, Inc., Cedar Park, TX*

ThP 355 **TOF-MS Ion Detector that Combines MCP and Avalanche Diode Achieves Higher Pulse Linearity and less than 1 ns Response Time**; Hiroshi Kobayashi[1]; Motohiro Suyama[1]; *[1]hamamatsu Photonics K.K., IWATA, Shizuoka*

ThP 356 **Development of the Triode-type MCP-based Compact Ion Detector for High Pressure Operation in Miniature Mass Spectrometer**; Masahiro Hayashi[1]; Yuuya Washiyama[1]; Joji Sakakiyama[1]; Hayato Inoue[2]; Toshiyuki Uchiyama[1]; *[1]Hamamatsu Photonics K.K., Iwata, Japan; [2]Hamamatsu Corporation, San Jose, CA*

ThP 357 **Pushing Limits in Native Mass Spectrometry: the Ultrahigh Mass Range Orbitrap Mass Spectrometer**; Kyle L. Fort[1]; Michiel van de Waterbeemd[1]; Dmitriy Boll[2]; Maria Reinhardt-Szyba[2]; Mikhail E. Belov[2]; Alexander A. Makarov[2]; Albert J. R. Heck[1]; *[1]Utrecht University, Utrecht; [2]Thermo Fisher Scientific, Bremen, Germany*

ThP 358 **The Implications of Detector Performance in GC/MS and LC/MS Analysis – Detectors Make the Difference!**; Nathan Contino[1]; Jeff Kernan[1]; Harry Prest[1]; Bjorn Flatt[1]; Bill Russ[1]; *[1]Agilent Technologies Inc., Santa Clara, CA*

ThP 359 **A Dual-Mode Detector with greatly Extended Dynamic Range and an HED**; Wayne Sheils[1]; Dick Stresau[1]; Kevin Hunter[1]; Peter Raffin[1]; Clifton Chey[1]; Alex Korenblium[1]; *[1]ETP Ion Detect, Clyde, Australia*

ThP 360 **Longevity Testing of a Prototype Discrete Dynode Detector for Triple Quadrupole Mass Spectrometer**; Oleg Silivra[1]; Michael Ugarov[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

ThP 361 **Implementation of Dual Detection Method for Miniaturized Time of Flight Mass Spectrometers**; Linxia Song[1]; Stephanie Mengis[1]; Theresa Evans-Nguyen[1]; *[1]University of South Florida, Chemistry department, Tampa , Florida*

ThP 362 **Ultra High Resolution MS Aids Unknown Extractable Component Identification**; Kate Comstock[1]; Seema Sharma[1]; Jesse D. Canterbury[1]; Vlad Zabrouskov[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

ThP 363 **Mass Analyzing Cold Ions in a Cryogenic Linear Ion Trap**; Larry Tesler[1]; Nicolas C Polfer[1]; *[1]University of Florida, Department of Chemistry, Gainesville, FL*

ThP 364 **Development of a Ultrahigh Resolution Multi-reflection Time-of-Flight Mass Spectrometer for Native Mass Spectrometry**; Keyong Hou[1]; Ping Chen[1]; Jichun Jiang[1]; Haiyang Li[1]; *[1]Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China*

ThP 365 **The sTOF, a Favorable Geometry for a Time-Of-Flight Analyzer**; Daniel Murphy; *NOAA, Boulder, CO*

ThP 366 **A Modular Ion Funnel for Improved Sensitivity in Proton-Transfer-Reaction – Time-Of-Flight Mass Spectrometry (PTR-TOFMS) Instruments**; Alfons Jordan[1]; Christian Lindinger[1]; Stefan Feil[1]; Paul Mutschlechner[1]; Gernot Hanel[1]; Eugen Hartungen[1]; Jens Herbig[1]; Lukas Maerk[1]; Philipp Sulzer[1]; Simone Juerschik[1]; *[1]IONICON Analytik GmbH, Innsbruck, Austria*

ThP 367 **Controlling Kinetic Energies of Ions Radially Ejected from the Linear Ion Trap**; Viatcheslav V. Kovtoun; *Thermo Fisher Scientific, San Jose, CA*

ThP 368 **Coaxial Surface Induced Dissociation of Mass-Selected Ions**; Xinwei Liu[1]; Xiaoyu Zhou[1]; Zheng Ouyang[1, 2]; *[1]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instruments, Tsinghua University, Beijing, China; [2]Weldon School of Biomedical Engineering and Department of Chemistry, Purdue University, West Lafayette, IN*

ThP 369 **Particle-in-Cell Simulation of Quadrupolar Ion Detection in the NADEL Cell with Four Detection Electrodes**; Joshua Driver[1]; I. Jonathan Amster[1]; Andriy Kharchenko[2, 3]; Konstantin O. Nagornov[4]; Anton N. Kozhinov[4]; Yury O. Tsybin[4]; *[1]University of Georgia, Athens, GA; [2]University of Georgia, Athens, Georgia; [3]NAS Institute of Cybernetics, Kyiv, Ukraine; [4]Spectroswiss Sàrl, Lausanne, Switzerland*

ThP 370 **Effect of the Parametric Resonance Suppression and its Use in Linear Ion Tap Mass Spectrometry**; Mikhail Sudakov[1]; Igor Filippov[2]; *[1]SIMAX-MS, St.Petersburg, Russia; [2]MSCUBE, Auckland, New Zealand*

ThP 371 **Periodic Auxiliary AC Frequency Scanning for Rapid Mass Spectrometry Analysis**; Xinming Huo[1]; Fei Tang[1]; *[1]Tsinghua University, Beijing*

ThP 372 **Comprehensive Modeling and Experimental Validation of Ultrahigh Mass Resolution Linear Time-Of-Flight Mass Spectrometry**; Yu-Meng Ou[1, 2]; Yin-Hung Lai[1]; Yi-Hong Cai[1]; Chih-Hao Hsiao[1]; Cheng-Kai Jan[1]; Huan-Tsung Chang[2]; Yi-Sheng Wang[1]; *[1]Genomics Research Center Academia Sinica, Taipei; [2]Department of Chemistry, National Taiwan University, Taipei, Taiwan*

ThP 373 **Right Angle Ion Mirror-Prism (RAIMP): Mass Analyzer Combining Slit Spectroscopy with Retarding Electric Fields**; Igor V. Veryovkin[1]; Luke Hanley[1]; *[1]University of Illinois at Chicago (UIC), Chicago, IL*

ThP 374 **Determination of Ion Secular Frequency Bandwidth in Micro Ion Trap High Pressure Mass Spectrometers**; Gregory F. Brabeck[1]; J. Michael Ramsey[1]; *[1]UNC - Chapel Hill, Chapel Hill, NC*

ThP 375 **Minimization of Combined Magnetic and Electric Residual Fields to Further Improve the Resolution and Sensitivity in FTICR-MS**; Qinghao Wu[1]; Jared B Shaw[1]; Ljiljana Pasa-Tolic[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

ThP 376 **Improving the Precision of Quantitative Analysis for Linear Ion Trap Tandem Mass Spectrometry**; Linfan Li[1]; Cornelia L Boeser[1]; Jae C Schwartz[1]; John E Syka[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

ThP 377 **Analyzing Large Protein with High Resolution by AMS-200 series: inTrap MALDI Mass Spectrometer**; Shih-Chieh Yang[1]; Szu-Wei Chou[1]; Yao-Hsin Tseng[1]; Yi-Kun Lee[1]; Chih-kuang Chen[1]; Chun-Yen Cheng[1]; *[1]AcroMass technologies, Inc., Taipei*

ThP 378 **The Concept of 3D MR TOF Mass Spectrometry**; Yerbol Sapargaliyev[1, 2]; Aldan Sapargaliyev[2, 3]; *[1]REB, San Jose, Ca;*

[2]OiArna LLP, Almaty, Kazakhstan; [3]Nazarbayev University, Astana, Kazakhstan

ThP 379 **Buffer Gas Concentration Effects on Collisional Cooling in a Digital Ion Trap**; Timothy Vazquez[1]; Arik Townsend[2]; Theresa Evans-Nguyen[1]; *[1]University of South Florida, Tampa, FL; [2]University of South Florida, Tampa, FL*

ThP 380 **Improving Quadrupole Performance with a Thin DC Only Quadrupole Prefilter: Achieving High Performance in Tandem Mass Spectrometers with Reduced Size**; Laura L. Pollum[1]; Haopeng Wang[1]; Kenneth R. Newton[1]; James L. Bertsch[1]; Shane E. Tichy[1]; *[1]Agilent Technologies, Santa Clara, CA*

ThP 381 **CRAFTIEST: Cross Sectional Areas by Fourier Transform in Electrostatic Traps**; Eric T. Dziekonski[1]; Joshua T. Johnson[1]; Scott A McLuckey[1]; *[1]Purdue University, West lafayette, Indiana*

ThP 382 **The Application of Dual Channel High Speed Oscilloscope Analog-to Digital Converters to Time-of-Flight Mass Spectrometry**; Jennifer Sanderson[1]; August Hidalgo[2]; Kai Chen[2]; *[1]Agilent Technologies, Santa Clara, CA; [2]Agilent Technologies Inc., Santa Clara, CA*

ThP 383 **Characterization of Harmonic Signal Acquisition with Parallel Dipole and Multipole Detectors**; Sung-Gun Park[1]; James Bruce[1]; Gordon Anderson[2]; *[1]University of Washington, Seattle, WA; [2]GAA Custom Engineering, LLC, Benton, WA*

ThP 384 **Digital Waveform Technology and the Next Generation of Instrumentation**; Peter T. A. Reilly[1]; Katherine G. E. Donahoe[2]; Nathan Michael Hoffman[2]; Ashley Marie Moon[2]; Zachary Philip Gotlib[2]; Bojana Opacic[2]; Adam Paul Huntley[2]; *[1]Washington State University, Pullman, WA; [2]Washington State University, Pullman, WA*

ThP 385 **Characterization and Optimization of Toroidal Trapping Fields using Enhanced SIMION Tools**; Robert H. Jackson Iii[1]; David J. Manura[2]; Edgar D. Lee[3]; Stephen A. Lammert[3]; *[1]Instrumental Design Physics, LLC, Littleton, MA; [2]Scientific Instrument Services, Inc, Ringoes, NJ; [3]PerkinElmer, Inc, American Fork, UT*

ThP 386 **Digital Electrode Array for Compact Mass Analysis** ; Jerome Moore; *Robot Nose, Lemont, IL*

ThP 387 **Generation of Digital Waveforms with High Resolution Duty Cycle**; Nathan Michael Hoffman[1]; Zachary Philip Gotlib[1]; Brian Herbert Clowers[1]; Peter T. A. Reilly[2]; *[1]Washington State University, Pullman, WA; [2]Washington State University, Pullman, WA*

ION MOBILITY: FAIMS/DMS
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ThP 388 **Simultaneous, Rapid and High-Throughput Detection and Quantitation of Multiple Radiation Biomarkers in Human and Nonhuman Primate Urine by DMS-MS**; Zhidan Chen[1]; Stephen L. Coy[1]; Evan L. Pannkuk[2, 3]; Evagelia C. Laiakis[2]; Albert J. Fornace[2, 3]; Paul Vouros[1, 4]; *[1]Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA; [2]Department of Biochemistry and Molecular&Cellular Biology, Georgetown University, Washington, DC; [3]Tumor Biology Program, Lombardi Comprehensive Cancer Center, Georgetown University, Washington, DC; [4]Barnett Institute of Chemical and Biological Analysis, Northeastern University, Boston, MA*

ThP 389 **New FAIMS with Heated Electrospray Ionization (HESI) Source for High Chromatographic Flow Rate Application**; Satendra Prasad[1]; Michael Belford[2]; Rae Ana Snyder[2]; Susan E Abbatiello[3]; Jean-Jacques Dunyach[4]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]ThermoFisher Scientific, San Jose, CA; [3]Thermo Scientific, Cambridge, MA; [4]Thermo Fisher Scientific, San Jose, CA*

ThP 390 **A Novel Compact FAIMS Interface for Deeper Proteomic Analyses**; Sibylle Pfammatter[1]; Eric Bonneil[1]; Michael Belford[2]; Satendra Prasad[2]; Jean-Jacques Dunyach[2]; Pierre Thibault[1, 3]; *[1]IRIC-Université de Montréal, Montréal, QC, Canada; [2]ThermoFisher Scientific, San Jose, CA; [3]Departement Of Chemistry, Université de Montréal, Montréal, QC, Canada*

ThP 391 **Strategies for Improving FAIMS Performance for Clinical Applications**; Michael Wei[1]; Robin H.J. Kemperman[1]; Michael Costanzo[2]; Jared Boock[3]; Richard A. Yost[1]; *[1]University of Florida, Gainesville, FL; [2]Breathtec Biomedical, Inc., Gainesville, Florida; [3]Cannabix Technologies, Gainesville, Florida*

ThP 392 **Mitigating Fragmentation of Peptides with Controlled Clustering**; J.C. Yves Leblanc[1]; Brendon Seale[1, 2]; Bradley B Schneider[1]; Aaron Wheeler[2]; *[1]SCIEX, Concord, ON, Canada, ON, Canada; [2]University of Toronto, Toronto, ON, Canada*

ThP 393 **The Impact of Improved Selectivity through Enhanced Resolution and Field Asymmetric Ion Mobility on Defined Method LOQs and LODs**; Hans Schweingruber[1]; Michael Belford[1]; Satendra Prasad[1]; Susan E Abbatiello[1]; Claudia Martins[1]; Neloni Wijeratne[1]; Mary Blackburn[2]; *[1]ThermoFisher, San Jose, CA; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 394 **APPI-FAIMS-FTMS for the Investigation of Structural Features of Isomeric Crude Oil Constituents**; Alessandro Vetere[1]; Wolfgang Schrader[2]; *[1]Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany; [2]Max-Planck Inst für Kohlenforschung., Mülheim / Ruhr*

ThP 395 **How Mass Spectrometer Model and Electrode Temperature Determines FAIMS Separation**; Michael Belford[1]; Satendra Prasad[1]; Susan E. Abbatiello[2]; Hoa Pham[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Scientific, Cambridge, MA*

ThP 396 **Exploring the Separation of Phospholipids Using a Novel FAIMS Device in Conjunction with MS/MS Mode of Analysis**; Rae Ana Snyder[1]; Satendra Prasad[1]; Michael Belford[1]; *[1]Thermo Fisher Scientific, San Jose, California*

ThP 397 **Pre-Filtration of Transition Metals in Differential Mobility Spectrometry**; Ifeoluwa Ayodeji[1]; Theresa Evans-Nguyen[1]; Ronelle Bailey[1]; Christina Mancuso[1]; *[1]University of South Florida, Chemistry department, Tampa , FL*

ThP 398 **Separation of Triacylglycerol Positional Isomers in Plants Using Differential Mobility Spectrometry**; Jesse Balcer[1]; Jeffrey Gilbert[2]; Laura Wayne[2]; Yelena Adelfinskaya[2]; Scott Greenwalt[2]; Daniel Gachotte[2]; Lisa Buchholz[2]; *[1]Dow AgroSciences, Indianapolis, IN; [2]Dow AgroSciences, Indianapolis, IN*

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ThP 399 **Influence of Ionization Source Conditions on the Protomer Population Distribution of Anilinium and Related Cations**; Hanxue Xia; *SIT, jersey city, New Jersey*

ThP 400 **Towards Serpentine Ultra Long Ion Path for Enhanced Resolution Using Traveling Wave Structures for Lossless Ion Manipulations (SUPER TW-SLIM)** ; Ahmed Mohamed Hamid[1]; Sandilya V.B. Garimella[1]; Yehia M Ibrahim[1]; Liulin Deng[1]; Aneesh Prabhakaran[1]; Ian K Webb[1]; Gordon A Anderson[1]; Spencer A Prost[1]; Randolph V Norheim[1]; Jeremy A Sandoval[1]; Colby E Schimelfenig[1]; Erin S Baker[1]; Richard D. Smith[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

ThP 401 **Evaluation of Pulsed Nano-ESI Atmospheric Pressure Ion Mobility MS for Collision Cross Section Measurements**; William McMahon[1]; Rohan Dalvi[2]; Kaveh Jorabchi[1]; *[1]Georgetown University, Washington, DC; [2]Montgomery Blair High School, Silver Spring, MD*

ThP 402 **Supercritical Planar DMA P5 working at a resolving power of 110**; Mario Amo González[1]; Juan Fernandez de la Mora[2]; *[1]SEADM, Boecillo, Spain; [2]Yale University, New Haven, Connecticut*

ThP 403 **Structural Specificity of Ion Mobility Collision Cross Section for Characterization of Lipids**; Jody C. May[1]; Stacy D. Sherrod[1]; Katrina L Leaptrot[1]; Charles M. Nichols[1]; John A. McLean[1]; *[1]Center for Innovative Technology, Vanderbilt University, Nashville, TN*

ThP 404 **Simultaneous and Co-located Dual Polarity Ion Confinement and Separation in Traveling Wave-based Structures for Lossless Ion Manipulations (SLIM)**; Isaac K. Attah[1]; Sandilya V.B. Garimella[2]; Yehia M. Ibrahim[2]; Ian K. Webb[2]; Aneesh Prabhakaran[2]; Richard D. Smith[2]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Pacific Northwest National Laboratory, Richland, WA*

ThP 405 **Development of Ion-Mobility Orbitrap for Analysis of Large Proteins and Protein Complexes**; Michael Poltash[1]; David H Russell[1]; *[1]Texas A&M University, College Station, Texas*

ThP 406 **Ion Mobility Spectrometry of Foldamers and Foldaxanes. Optimization of Parameters Used for Theoretical CCS Calculation**; Frederic Rosu[1]; Yann Ferrand[1]; Victor Maurizot[1]; Ivan Huc[1]; Valérie Gabelica[2,3]; *[1]CNRS / Univ. Bordeaux, Pessac, France; [2]University of Bordeaux, Pessac, FR; [3]Inserm, Bordeaux, France*

ThP 407 **An Ion Mobility filter based on Structures for Lossless Ion Manipulations (SLIM)**; Aneesh Prabhakaran[1]; Ahmed Mohamed Hamid[2]; Yehia M Ibrahim[2]; Sandilya Garimella[2]; Robert G Ewing[2]; Blandina R Valenzuela[2]; Jeremy A Sandoval[2]; Richard D. Smith[2]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Pacific Northwest National Laboratory, Richland, WA*

ThP 408 **Collision Cross Section Measurement in Traveling Wave Ion Mobility Spectrometry: Analytical Comparison of Functions for Fitting Calibration Curves**; Alana L Rister[1]; Abby S Gelb[1]; Eric D Dodds[1]; *[1]University of Nebraska - Lincoln, Lincoln, NE*

ThP 409 **Correlating Resolving Power, Resolution, and Collision Cross Section: A Cross Platform Study of Separation Efficiency in Ion Mobility Spectrometry**; James Dodds[1]; Jody C. May[1]; John A. McLean[1]; *[1]Vanderbilt University, Nashville, TN*

ThP 410 **Collision Cross Section Calibration with Structures for Lossless Ion Manipulations Mixture Analysis by Traveling Wave Ion Mobility**; Ian K. Webb[1]; Liulin Deng[1]; Ahmed M Hamid[1]; Roza Wojcik[1]; Erin S Baker[1]; Yehia M Ibrahim[1]; Richard D. Smith[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

ThP 411 **Selective Ion-Neutral Clustering to Enhance Ion Mobility Separation Factors**; Pearl Kwantwi-Barima; *Washington State University, Pullman, WA*

ThP 412 **Optimization of Electron Capture Dissociation for the Analysis of Glycans, Peptides, and Proteins Using a IM-QTOF Mass Spectrometer**; James A. Hill[1]; Rebecca S. Glaskin[1]; Valery G. Voinov[2]; Joseph S. Beckman[2]; Catherine E Costello[1]; *[1]Boston University School of Medicine, Boston, MA; [2]e-MSion, Corvallis, OR*

ThP 413 **Accurate Absolute Collision Cross Sections *via* the "CRAFTI" FTICR Linewidth Technique**; Anupriya Anupriya[1]; Elaura Gustafson[1]; David V. Dearden[2]; *[1]Brigham Young University, Provo, UT; [2]Brigham Young University, Provo, UT*

ThP 414 **Determining the Upper-Mass Limit for Obtaining Accurate CRAFTI Collision Cross Section Measurements Using Variable Length Polyalanine Peptides**; Brigham Pope[1]; David V. Dearden[1]; Anupriya Anupriya[1]; *[1]Brigham Young University, Provo, UT*

ThP 415 **Identification of Isomers by Fingerprint Isotopic Fine Structure in High-Resolution FAIMS Spectra**; Julia L. Kaszycki[1]; Matthew A. Baird[1]; Andrew P. Bowman[1]; Alexandre Shvartsburg[2]; *[1]Wichita State University, Wichita, KS; [2]Wichita State University, Wichita, KS*

ThP 416 **Exploring Dendrimers as Calibrants for Ion Mobility-Mass Spectrometry**; Scott M. Grayson[1]; Michael Malkoch[2,3]; Jamie Godfrey[3]; Surinthra Mongkhontreerat[3]; Nick Tomczyk[4]; Jakub Ujma[4]; Kevin Giles[4]; *[1]Tulane University, New Orleans, LA; [2]KTH Royal Institute of Technology, Stockholm, Sweden; [3]Polymer Factory Sweden AB, Stockholm, Sweden; [4]Waters Corp., Wilmslow, UK*

ThP 417 **Conformational Dynamics in Ion Mobility Data**; Poyer Salomé[1]; Comby-Zerbino Clothilde[2]; Choi Chang Min[2]; MacAleese Luke[2]; Salpin Jean-Yves[1]; Dugourd Philippe[2]; Fabien Chirot[3]; *[1]LAMBE, Université Evry Val d'Essonne, CEA, CNRS, Université Paris-Saclay, Evry, France; [2]Institut Lumière Matière, Université de Lyon, Université Lyon 1, CNRS, Lyon, France; [3]Institut des Sciences Analytiques, Université de Lyon, Université Lyon 1, Ens de Lyon, CNRS, Lyon, France*

ThP 418 **Quantitative Ion Mobility-Mass Spectrometry for Identifying Protein/Peptide Conformation/Multimer Ions**; KENT GILLIG[1]; Chung-Hsuan Chen[1]; *[1]Academia Sinica, Taipei, Nankang, Section 2, Taipei 115*

ThP 419 **Collision Cross Sections of Polyoxometalates : Linking Experimental and Theoretical Values**; Sébastien Hupin[1]; Hélène Lavanant[1]; Madeleine Piot[2]; Guillaume Izzet[2]; Carlos Afonso[1]; *[1]Normandie Univ., UNIROUEN, INSA Rouen, CNRS, COBRA, 76000 Rouen, France; [2]Institut Parisien de Chimie Moléculaire UMR CNRS 8232, Sorbonne Universités, UPMC-Paris 6, 4 Place Jussieu, 75005 Paris, France*

ThP 420 **New Developments in Gated Trapped Ion Mobility Spectrometry for Coupling with FT-ICR Mass Analyzers**; Mark Ridgeway[1]; Mel Park[1]; *[1]Bruker Daltonics Inc., Billerica, MA*

ThP 421 **True vs. Average Mobility. New developments in Ion Mobility Separation**; Carlos Larriba Andaluz[1]; Tianyang Wu[2]; *[1]IUPUI, Indianapolis, IN; [2]IUPUI, Indianapolis, IN*

ThP 422 **A Comparison of Collision Cross Section Calibrants for Traveling Wave Ion Mobility Spectrometry Reveals Significant Discrepancies between Molecular Classes**; Eric D. Dodds[1]; Alana L. Rister[1]; Abby S. Gelb[1]; *[1]University of Nebraska - Lincoln, Lincoln, NE*

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ThP 423 **Improving Routine Analysis of Glycan Profiles in a QC Environment Using Spectral Libraries**; Brooke M Koshel[1]; Ximo Zhang[1]; Robert Birdsall[1]; Joe Fredette[1]; Min Du[1]; Ying Qing Yu[1]; *[1]Waters Corporation, Milford, MA*

ThP 424 **High-Throughput Comprehensive Analysis of Trace D- and L- Amino Acids Using Extra-Facile Chiral Separation and Column Switching**; Yuki Uno[1]; Toshikazu Minohata[1]; Jun Watanabe[1]; Hidetoshi Terada[1,2]; Junko Iida[1,2]; Yosuke Nakano[3]; Eiichiro Fukusaki[2,3]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Osaka University Shimadzu Analytical Innovation Research Laboratory, Graduate School of Engineering, Osaka University, Suita, Japan; [3]Department of Biotechnology, Graduate School of Engineering, Osaka University, Suita, Japan*

ThP 425 **Open Data Standard for LC/MS Data, Methods, and Results**; David Peterson[1]; Heiko Fessenmayr[2]; *[1]Agilent Technologies Inc., Santa Clara, California; [2]Agilent Technologies, Inc., Santa Clara, CA*

ThP 426 **Taking Nano Liquid Chromatography Coupled to Mass Spectrometry One Step Closer to the Clinics**; Ole Kristian Brandtzaeg[1]; Meire Ribeiro da Silva[1,2]; Tore Vehus[1]; Hanne Roberg-Larsen[1]; Elsa Lundanes[1]; Steven Ray

Wilson[1]; *[1]University of Oslo, Oslo, Oslo; [2]Universidade de São Paulo - USP, Sao Paulo, Brazil*

ThP 427 **Determination of Isoflavones in Dietary Supplements: a Comparison of Mass Detection with UV Detection**; Jinchuan Yang[1]; Mark Benvenuti[1]; Kenneth Rosnack[1]; Ramesh P Rao[2]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, UK*

ThP 428 **High-Throughput Strategies for Label-Free and SILAC LC-MS/MS Proteomics**; Yuan-wei David Nei[1]; Rey Redha[1]; Carrie E. Romer[1]; Jamie L. Allen[2]; Danielle B. Gutierrez[2]; Tina Tsui[2]; Michael R Heaven[3]; Jeremy L. Norris[2]; Richard M. Caprioli[2]; *[1]MSRC Vanderbilt University, Nashville, TN; [2]MSRC Vanderbilt University, Nashville, TN; [3]Vulcan Analytical, LLC, Birmingham, AL*

ThP 429 **Discovery Ion Current - A Novel Approach to Plot Total Ion Current Real-Time by Enhancing Signal from Newly Detected Ions**; Lawrence Klecha[1]; Daniel Eikel[1]; *[1]Advion Inc., Ithaca, NY*

ThP 430 **Selectivity Comparison of BromoBenzyl(PBr) to FluoroPhenyl(PFP) Core-Shell HPLC Columns**; Ken Tseng[1]; Toshi Ono[1]; Tsunehisa Hirose[2]; *[1]Nacalai USA, San Diego, CA; [2]Nacalai Tesque, Kyoto, Japan*

ThP 431 **How Combined New Approaches Can Improve Quantitative and Qualitative LC-MS**; Stephan Altmaier[1]; Hans Griesinger[1]; Michael Schulz[1]; *[1]Merck KGaA, Darmstadt, Germany*

ThP 432 **Spectrum Evaluation for the 2017 Released NIST Tandem MS Library**; Yuxue Liang[1]; Pedatsur Neta[2]; Xiaoyu Yang[2]; Stephen E Stein[2]; *[1]National Institute of Standards and Technology, Gaithersburg, MD; [2]National Institute of Standards and Technology, Gaithersburg, MD*

ThP 433 **Measurement of Amino Acid Modification after Fast Photochemical Oxidation of Proteins Utilizing Online Low-Flow Size Exclusion Chromatography**; Sandeep K Misra[1]; Joshua S. Sharp[1]; *[1]University of Mississippi, Oxford, MS*

ThP 434 **Chromatographic Behaviour of PTM-Carrying Peptides in Proteomic Experiments (RPLC, HILIC, CZE)**; Vic Spicer[1]; Haley Neustaeter[1]; Evelyn Ang[1]; Ying Lao[1]; Helene Perreault[1]; Oleg V. Krokhin[2]; *[1]University of Manitoba, Winnipeg, MB; [2]University of Manitoba, Winnipeg, MB*

ThP 435 **Automated Targeted Screening of Leachables in Pharmaceutical Drug Products by Single Quadrupole Mass Spectrometer System**; Syed Salman Lateef[1]; Siji Joseph[1]; *[1]Agilent Technologies India, Bangalore, India*

ThP 436 **Method for Quick and Efficient Packing of 50 cm Capillary Liquid Chromatography Columns for Mass-Spectrometry Based Proteomics**; Sergey I. Kovalchuk[1]; Wojciech Michalak[1]; Adelina Rogowska-Wrzesinska[1]; Ole N. Jensen[1]; *[1]Univ. Southern Denmark, Odense, Denmark*

ThP 437 **Eliminating a Common Yet Obscure Noise Source in LCMS and ICPMS** ; Robert Cunico[1]; Michael J Pinkerton[1]; Steve Graham[1]; *[1]ASI, Inc., Richmond, CA*

ThP 438 **2D-LC/MS Analysis of Fosfomycin Trometamol and Related Substances in Stress Testing Solvent**; Nan Hu[1]; Xialong Zuo[1]; *[1]Agilent Technologies, Beijing, China*

ThP 439 **Revealing Hidden Impurities in Bio-Pharmaceuticals by Multi-Dimensional Chromatography Preceding ESI-MS**; Stephan Buckenmaier [1]; Dwight Stoll[2]; Patrik Petersson[3]; *[1]Agilent, Waldbronn , Baden-Wuerttemberg; [2]Gustavus Adolphus College, Saint Peter, MN; [3]Novo Nordisk A/S, Måløv, Denmark*

ThP 440 **Toward Rapid Structure Elucidation of Cyclic Peptide Late Stage Functionalization using UPLC-HRMS with Customizable Reaction-Driven Data Processing**; Jason Hoar[1]; Fabien Fontaine[2]; Mikhail Reibarkh[1]; Yong Liu[1]; Ismael Zamora[2]; Shane Krska[1]; Christopher Sinz[1]; Kevin Bateman[1]; *[1]Merck & Co., Inc, Rahway, NJ; [2]Molecular Discovery, London, UK*

ThP 441 **The Development of a Method for the Determination of Cortisol and 6-Beta-Hydroxycortisol in Human Urine Using 2-D Chromatography**; Jeff Jeppson[1]; Elizabeth Dibbern[1]; Ridha Nachi[1]; Curtis Sheldon[1]; *[1]Celerion, Lincoln, NE*

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ThP 443 **Dynamic and Temporal Assessment of Human Dried Blood Spot MS/MSALL Shotgun Lipidomics Analysis**; Fei Gao[1]; Justice McDaniel[1]; Emily Y Chen[1]; Hannah Rockwell[1]; Jeremy Drolet[1]; Vivek K Vishnudas[1]; Vladimir Tolstikov[1]; Rangaprasad Sarangarajan[1]; Niven R Narain[1]; Michael A Kiebish[1]; *[1]Berg, LLC, Framingham*

ThP 444 **Elongation of Very Long Chain Fatty Acids (ELOVL) Isozymes Activity – A Lipidomics Approach Using Infusion-Based MS/MSALL**; Goncalo Vale[1]; Matthew Mitsche[1]; Bonne Thompson[1]; Kaitlyn Eckert[1]; Alex Treacher[1]; William Trenfield[1]; Young-ah Moon[1]; Jeffrey McDonald[1]; *[1]UT Southwestern, Dallas, TX*

ThP 445 **LC-MS Analysis of Lipids Nanoparticles (LNPs): One Shot, Four Lipids**; jiang qian[1]; Kanwaldeep Gill[1]; Zi Wang[1]; *[1]GSK Vaccines, Rockville, MD*

ThP 446 **Comparison of Eight High-Resolution LC-MS Platforms Validates Accurate Quantifications in Untargeted Plasma Lipidomics**; Tomas Cajka[1]; Jennifer T Smilowitz[2, 3]; Oliver Fiehn[1]; *[1]NIH West Coast Metabolomics Center, University of California Davis, Davis, CA; [2]Department of Food Science and Technology, University of California Davis, Davis, CA; [3]Foods for Health Institute, University of California Davis, Davis, CA*

ThP 447 **Development of an Integrated Workflow for Profiling and Semi-Quantitative Analysis of Lipids** ; Sheher Bano Mohsin[1]; Kevin Williams[2]; Durairaj Renu[3]; Ningombam Sanjib Meitei[4]; Shyam Kalakoti[3]; Stephen Madden[5]; *[1]Agilent Technologies Inc., Wood Dale, IL; [2]UCLA, Los Angeles, California; [3]Strand Life Sciences, Bengaluru, India; [4]PREMIER Biosoft, Indore, India; [5]Agilent Technologies Inc., Santa Clara, California*

ThP 448 **Investigating the Lipidomic Dynamics of Torpor through Examination of Hibernating Squirrel Liver Tissue and Dehydrated Frog Leg Tissue**; Katrin Blank[1]; Sam Williamson[1]; Hillary Weinert[1]; Carlos R. Canez[1]; Kenneth Storey[1]; Jeffrey C. Smith[1]; *[1]Carleton University, Ottawa, ON, Canada*

ThP 449 **Structural Characterization of Bioactive Fatty Acid Isomers Using Liquid Chromatography–Differential Mobility Spectrometry and Electron-Induced Dissociation Mass Spectrometry (LC-DMS-EID)**; Kazutaka Ikeda[1, 2]; Shuh Yasuda[1]; Yuuya Senoo[1]; Makoto Arita[1, 2, 3]; J. Larry Campbell[4]; J.C. Yves Leblanc[4]; Paul Rs Baker[5]; Takashi Baba[4]; *[1]RIKEN Center for Integrative Medical Sciences, Yokohama, Japan; [2]Yokohama City Univ., Yokohama, Japan; [3]Keio University, Tokyo; [4]SCIEX, Concord, ON, Canada; [5]SCIEX, Redwood City, CA*

ThP 450 **Development of a High-Sensitivity Method for Lipidomics of Small Volumes of Biological Fluids by nanoLC-MS**; Adriana Zardini Buzatto[1]; Jaspaul Tatlay[1]; Brian Kwon[2]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB, Canada; [2]University of British Columbia, Vancouver, BC, Canada*

ThP 451 **Investigation of Brain Tumors by Online Liquid Extraction Combined with ESI Ionization and Ultrahigh Resolution FTICR Mass Spectrometry**; Igor Popov[1, 2, 3];

Evgeny Zhvansky[1]; Vsevolod Shurhkhay[1, 4]; Nikita Levin[1]; Alexey Kononikhin[1, 2]; Anatoly Sorokin[1]; Oleg Kharybin[5]; Yury Kostyukevich[1, 5]; Maria Indeykina[1, 2, 3]; Alexander Potapov[4]; Eugene (Evgeny) Nikolaev[1, 2, 5]; *[1]Moscow Institute of Physics and Technology (State University), Dolgoprudnyj, Russia; [2]Institute for Energy Problems of Chemical Physics of RAS, Moscow, Russia; [3]Emanuel Institute of Biochemical Physics of Russian Academy of Sciences, Moscow, Russia; [4]N. N. Burdenko Scientific Research Neurosurgery Institute, Moscow, Russia; [5]Skolkovo Institute of Science and Technology, Skolkovo, Russia*

ThP 452 **Characterizing Human Meibum by Shotgun Lipidomics, MS/MSall and Successive Polarity Switching**; Jianzhong Chen[1]; Kelly K Nichols[2]; *[1]University of Alabama at Birmingham, Birmingham, AL; [2]University of Alabama at Birmingham, Birmingham, AL*

ThP 453 **Acoustically-induced Electrospray Mass Spectrometry of Extracellular Vesicle Lipids**; Xabier Osteikoetxea[1]; Martin Bachman[1]; Ian Sinclair[1]; Nikki Heath[1]; Lois Grant[1]; Jonathan Wingfield[2]; Niek Dekker[3]; Ross Overman[1]; *[1]AstraZeneca R&D, Alderley Park, UK; [2]AstraZeneca R&D, Cambridge, UK; [3]AstraZeneca R&D, Gothenburg, Sweden*

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ThP 454 **Open-Source Lipidomics Software for Rapid Semi-Quantification and Visualization**; Jason A. Cochran[1]; Jeremy Koelmel[2]; John A. Bowden[3]; Richard A Yost[2]; Timothy J. Garrett[2, 4]; *[1]University of Florida, College of Engineering, Gainesville, FL; [2]University of Florida, Department of Chemistry, Gainesville, FL; [3]National Institute of Standards and Technology, NIST, Hollings Marine Laboratory, Charleston, SC; [4]University of Florida, Clinical and Translational Science Institute, Gainesville, FL*

ThP 455 **A Novel LC-MS/MS Method for Ganglioside Profiling of Glaucoma Disease in Mice**; Ashta Lakshmi Prasad Gobburi[1]; Denise Inman[2]; David J Anderson[1]; *[1]Cleveland State University, Department of Chemistry, Cleveland, OH; [2]Northeast Ohio Medical Univeristy, Rootstown, Ohio*

ThP 456 **Challenges for the Quantification of DMG-PEG GM-020 in Mouse Plasma by HPLC-MS/MS**; Lijuan Fu[1]; Bryce Ashby[1]; Shawn Burton[1]; Qian Guo[1]; Scott Reuschel[1]; Min Meng[1]; Aihua Liu[1]; *[1]Covance, Salt Lake City, UT*

ThP 457 **High Throughput Lipid Identification and Quantification Using a Directed HRAM LC-MS-MS approach on a Modified Quadrupole-Orbitrap Mass Spectrometer** ; Reiko Kiyonami[1]; David Peake[1]; Andreas F. Huhmer[1]; *[1]ThermoFisher Scientific, San Jose, CA*

ThP 458 **Locating Apolipoprotein A2 Protein in the Central Nervous System**; Sausan Azzam[1, 2]; Xiaolin Li[1, 2]; Mark R. Chance[1, 2]; Kingman P. Strohl[3]; *[1]Center for Proteomics and Bioinformatics, Case Western Reserve University, Cleveland, OH; [2]Department of Nutrition, Case Western Reserve University, Cleveland, OH; [3]Department of Medicine, University Hospitals Case Medical Center, Cleveland, OH*

ThP 459 **Development of an HILIC Based LC-MS/MS for High-Throughput Targeted Lipidomics**; Junhua Wang[1]; Mackenzie Pearson[1]; Paul Rs Baker[1]; *[1]SCIEX, Redwood City, CA*

ThP 460 **Identification and Quantification of Esterified Hepoxilin A3 in the ileum of Mice after Total Body Irradiation Using Oxidative Phospholipidomics**; Yulia Y Tyurina[1]; Vladimir A Tyurin[1]; Andrew A Amoscato[1]; Tami Anthonymuthu[1]; Michael W Epperly[1]; Simon S Watkins[1]; Joel S Greenberger[1]; Hülya Bayir[1]; Valerian E Kagan[1]; *[1]University of Pittsburgh, Pittsburgh, PA*

ThP 461 **Towards Quantitative Analysis of MALDI Mass Spectral Data Using linear Poisson Independent Component Analysis**; Somrudee Deepaisarn[1]; Adam McMahon[1]; Neil A. Thacker[1]; Paul D. Tar[1]; Ashley Seepujak[1]; *[1]University of Manchester, Manchester, UK*

ThP 462 **Dysregulated Lipid Profiles of Non-Alcoholic Fatty Liver Disease (NAFLD)**; Timothy J Garrett[1]; Rainey E Patterson[2]; Baljit Ubhi[3]; Ken Cusi[4]; *[1]Univ of Florida, Gainesville, FL; [2]Eastman Chemical Company, Kingsport, TN; [3]SCIEX, Redwood City, CA; [4]University of Florida, Gainesville, FL*

ThP 463 **Cardiolipin Remodeling in the Developing Brain after Trauma**; Tamil S Anthonymuthu[1]; Honglu Chao[2, 3]; Andrew A Amoscato[2]; Jing Ji[3]; Valerian E Kagan[2]; Hülya Bayır[2]; *[1]University Of pittsburgh, Pittsburgh, PA; [2]University of Pittsburgh, Pittsburgh, PA; [3]Nanjing Medical University, Nanjing, China*

ThP 464 **The Unusual Ionization Behavior of Ceramides on Sciex 6500QTRAP Instrument during LC-MS/MS Analyses**; Irina Bronova[1]; John Jung[1]; Evgeny Berdyshev[1]; *[1]National Jewish Health, Denver, CO*

ThP 465 **Untargeted Metabolomic Analysis of omega-3 Ethyl Ester Supplementation**; Stacy Gelhaus[1]; Francisco J. Schopfer[1]; Sonia R. Salvatore[1]; Carsten Skarke[2]; *[1]Univ of Pittsburgh, Pittsburgh, PA; [2]University of Pennsylvania, Philadelphia, PA*

ThP 466 **Novel Method for Total Butyrate Quantification in Human Milk Using GC-MS**; Stephanie P. Shu[1]; Judy Cundiff[1]; Michael Gray[1]; Sarah Maria[1]; Shay Phillips[1]; Ardythe L. Morrow[2]; *[1]Mead Johnson Nutrition, Evansville, IN; [2]Cincinnati Children's Hospital Medical Center, Cincinnati, OH*

ThP 467 **Contribution of Biosynthesis vs Remodeling to the Diversity of Cardiolipins in Genetically and Nutritionally Manipulated Yeast Cells: Differential LC-MS Assessments**; Vladimir A. Tyurin[1]; Yulia Y. Tyurina[1]; Wenjia Lou[2]; Feng Qu[1]; Jenney Liu[3]; Maik Hüttemann[3]; Dariush Mohammadyani[1, 4]; Michael A. Frasso[1]; Peter Wipf[1]; Hülya Bayir[1]; Miriam L. Greenberg[3]; Valerian E. Kagan[1]; *[1]University of Pittsburgh, Pittsburgh, PA; [2]Wayne State University, Detroit , MI; [3]Wayne State University, Detroit, MI; [4]Johns Hopkins University, Baltimore, MA*

ThP 468 **Diagnostic Evaluation of Steroidomics in a Breast Cancer Cohort in Sweden by Convergence Chromatography-Tandem Mass Spectrometry**; Neil De Kock[1]; Kumari Ubhayasekera[1]; Jonas Bergquist[1]; *[1]Uppsala University, Uppsala , Sweden*

ThP 469 **Optimization of LC-ESI-MS Methods for Targeted and Semi-Targeted Screening of N-acyl Phosphatidylethanolamines in Mouse Brain Tissue**; Theresa Mclaughlin[1]; Ludmila Alexandrova[2]; Allis Chien[2]; *[1]Stanford University, Palo Alto, CA; [2]Stanford University, Stanford, CA*

ThP 470 **Quantitative Analysis of Bis(monoacylglycero) phosphate and Phosphatidylglycerol Isomers by Shotgun lipidomics after One-step Methylation**; Miao Wang[1]; Xianlin Han[1]; *[1]Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL*

ThP 471 **A Miniaturized LC-MS/MS Platform for In-Depth Quantitative Profiling of Endocannabinoids and Related N-Acylethanolamines in Human Cerebrospinal Fluid**; Vasudev Kantae[1]; Shinji Ogino[1]; Marek Noga[1]; Amy C Harms[1]; Robin M. van Dongen[2]; Gerrit L. J. Onderwater[2]; Arn M. J. M. van den Maagdenberg[2]; Gisela M. Terwindt[2]; Mario van der Stelt[1]; Michel D. Ferrari[2]; Thomas Hankemeier[1]; *[1]Leiden University, Leiden, Netherlands; [2]Leiden University Medical Center, Leiden, Netherlands*

ThP 472 **Accumulation of Oxygenated Phosphatidylethanolamines as Ferroptotic Death Signals Characterized by Oxidative Phospholipidomics**; Feng Qu[1]; Yulia Y Tyurina[1]; Jinming Zhao[2]; Gaowei Mao[3]; Vladimir A Tyurin[1]; Tami Selvan Anthonymuthu[3]; Andrew A Amoscato[1]; David R Emlet[3]; John A Kellum[3]; Sally E Wenzel[2]; Hülya Bayir[3]; Valerian E Kagan[1]; *[1]Departments*

of Environmental and Occupational Health, University of Pittsburgh, Pittsburgh, PA; [2]Department of Medicine, University of Pittsburgh, Pittsburgh, PA; [3]Department of Critical Care Medicine, University of Pittsburgh, Pittsburgh, PA

ThP 473 **Global Profiling of FPP/GGPP-Protein Interactome in Liver *via* BSS-based Affinity Purification and Mass Spectrometry**; Jingzi Zhang[1, 2]; Lei Fang[1, 2]; Chaojun Li[1, 2]; *[1]The Medical School of Nanjing University, Nanjing, China; [2]Model Animal Research Centre of Nanjing University, Nanjing, China*

ThP 474 **Lipidomic Profiling of Targeted Oxylipins in Human Plasma with Ultra-Performance Liquid Chromatography-Tandem Mass Spectrometry** ; Zhi-Xin Yuan[1]; Christopher E Ramsden[1]; *[1]Lipid Mediators, Inflammation and Pain Unit, Laboratory of Clinical Investigation, National Institute on Aging, NIH., Bethesda, MD*

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ThP 475 **MALDI-MS/MS to Determine Sequencing Information of Novel Side Chain Liquid Crystalline Copolymers**; Savannah Snyder[1]; Huiming Xiong[2]; Chrys Wesdemiotis[3]; *[1]The University of Akron, Akron, Ohio; [2]Shanghai Jiao Tong University, Shanghai, China; [3]The University of Akron, Akron, OH*

ThP 476 **Nanoparticle Microarray for High-Throughput Microbiome Metabolomics Using Nanoparticle-Assisted Laser Desorption Ionization Mass Spectrometry**; Maria Emilia Dueñas[1]; Rebecca Hansen[1]; Young-Jin Lee[1]; *[1]Iowa State University, Ames, IA*

ThP 477 **Development of a Nanodiamond-based Multifunctional Platform for Bacteria Sensing, Identification, and Disinfection**; Chih-Che Wu; *Department of Applied Chemistry, National Chi Nan University, Puli, Taiwan*

ThP 478 **AP-MALDI-Q-IMS-TOF MS as a Liquid Sample Mass Profiling Platform for Food Authenticity Tests**; Oliver John Hale[1]; Michael Morris[2]; Rainer Cramer[1]; *[1]University of Reading, Reading, UK; [2]Waters Corporation, Wilmslow, UK*

ThP 479 **Imaging Nanoparticle Drug Delivery Systems, their Cargo, and their Effect on Tissue Biochemistry by MALDI-MS**; Kristen Sikora[1]; Laura Castellanos[1]; Ying Jiang[1]; Joseph Hardie[1]; Vincent M Rotello[1]; Richard W Vachet[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

ThP 480 **Investigation of the Binding Character of Potential Five Lipoxygenase Enzyme Inhibitors with On-Target Incubation**; Michael Ruehl[1]; Benjamin Kuehn[1]; Ute Bahr[1]; Bettina Hofmann[1]; Dieter Steinhilber[1]; Michael Karas[1]; *[1]Goethe-University, Frankfurt am Main, Germany*

ThP 481 **Electron Transfer Ionization in MALDI-MS Using π-Extended Fluorenes as Matrices**; Juan S. Ramirez[1]; Cristian Blanco-Tirado[1]; Marianny Y. Combariza[1]; *[1]Universidad Industrial de Santander, Bucaramanga, Colombia*

ThP 482 **Cholesterol, Phospholipids and Glucose Detection in Vitreous Humor from Diabetic Human Donors**; Abigail Schnepf[1]; M Cecilia Yappert[1]; Douglas Borchman[1]; *[1]University of Louisville, Louisville, KY*

ThP 483 **MALDI MS Profiling of Serum Extracts to Identify Galactomannan Enzyme Immunoassay False Positivity *via* Immunoglobulin Products**; Matthew E. Openshaw[1]; Tom K. Abban[1]; Rebecca Gorton[2]; Simona Salivo[1]; Ekta Patel[1]; Emanuele Barborini[3]; Timothy D. McHugh[4]; Emmanuel Wey[4, 5]; *[1]Shimadzu, Manchester, UK; [2]Health Services Laboratories (HSL), London, UK; [3]Tethis SpA, Milan, Italy; [4]Centre for Clinical Microbiology, Division of Infection and Immunity, University College London, London, UK; [5]Royal Free London NHS Trust Department of Clinical Microbiology, London, UK*

ThP 484 **Identification of Lipid Biomarkers of Human Inflammatory Bowel Disease Using Imaging Mass Spectrometry**; Ekta Patel[1]; Simona Salivo[1]; Roberto Fernández[2]; Joan Bestard-Escalas[3]; Jone Garate[2]; Albert Maimó-Barceló[3]; Daniel H. López[3]; Sam Khorrami[3, 4]; Daniel Ginard[3, 4]; Gwendolyn Barceló-Coblijn[3]; José A. Fernández[2]; *[1]Shimadzu, Manchester, UK; [2]Dep. of Physical Chemistry, Fac. of Science and Technology, University of the Basque Country (UPV/EHU), Barrio Sarriena, Spain; [3]Research Unit, Hospital Universitari Son Espases, Institut d'Investigació Sanitària de Palma (IdISPa), Palma, Spain; [4]Gastroenterology Unit, Hospital Universitari Son Espases, Palma, Spain*

ThP 485 **Study of Oxidative Damage from Radiotherapy in HCT-116 Spheroids by MALDI Imaging**; Amaia Carrascal Minino[1]; Fiona Henderson[1]; Somrudee Deepaisarn[1]; Kaye J Williams[2]; Adam McMahon[1]; *[1]Wolfson Molecular Imaging Centre, CRUK/EPSRC Imaging Centre of Cambridge & Manchester, The University of Manchester, Manchester, UK; [2]Manchester Pharmacy School, University of Manchester, Manchester, UK*

ThP 486 **Analysis of Chlorophylls in Spinach (*Spinacia oleracea*) by Electron Transfer Ionization**; Juan S. Ramirez[1]; Yoleisy Orduz[1]; Julio R. Pinzón[1]; Cristian Blanco-Tirado[1]; Marianny Y. Combariza[1]; *[1]Universidad Industrial de Santander, Bucaramanga, Colombia*

ThP 487 **FTICR MALDI Analysis for Protein Footprinting and for Probing the Interaction of Warfarin with Vitamin K Epoxide Reductase**; Jerry Jiang; *Washington University in St. Louis, St. Louis, MO*

ThP 488 **A Simplified Expedited Screening of Haemoglobinopathy and Pre-Diabetes in Whole Blood Using MALDI MS**; Tom K. Abban[1]; Suzanne M. Docherty[2, 3]; Jason K. Iles[3, 4]; Simona Salivo[1]; Matthew E. Openshaw[1]; Ray K. Iles[3]; *[1]Shimadzu, Manchester, UK; [2]Department of Haematology, Addenbrookes Hospital, Cambidge, UK; [3]MAP Sciences Ltd, Bedford, UK; [4]Department of Biotechnology and Chemical Engineering University of Cambridge, Cambidge, UK*

ThP 489 **Clinical Top-down Proteomics for Rapid Detection and Isotyping of Monoclonal Gammopathies**; Surendra Dasari[1]; John R. Mills[1]; Mindy C. Kohlhagen[1]; David R. Barnidge[1]; Angela Dispenzieri[1]; David L. Murray[1]; *[1]Mayo Clinic, Rochester, MN*

ThP 490 **Sweet Beats! N-Glycan Changes in Allograft and Xenograft Heart Valves by MALDI Imaging Mass Spectrometry**; Peggi Angel[1]; Anna Biemann[2]; Connor West[1]; Kacey Talbot[1]; Richard R Drake[1]; Elizabeth Greene[3]; Lia H. Campbell[3]; Ulrich A Stock[2]; Kelvin Brockbank[3]; *[1]Medical University of South Carolina, Charleston, SC; [2]Royal Brompton and Harefield Foundation Trust, Imperial College, and Magdi Yacoub Institute, London, UK; [3]Tissue Testing Technolgoies, LLC, Charleston, SC*

ThP 491 **Optimized MALDI-TOF Mass Spectrometry Workflow for Biomarker Discovery in Unfractionated Serum**; Maximilian Steers[1]; Alex Nickel[1]; Nicholas Dupuis[1]; Gary Pestano[1]; *[1]Biodesix Inc, Boulder, CO*

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ThP 492 **Systemic Approaches for Understanding Regulatory Mechanisms Underlying Cancer Metabolism**; Iqbal Mahmud[1]; Guimei Tian[1]; Lisa Zhao[1]; Timothy J. Garrett[2]; Daiqing Liao[1]; *[1]University of Florida, Gainesville, FL; [2]University of Florida, Department of Immunology, Pathology, and Laboratory Medicine, Gainesville, FL*

ThP 493 **Mapping of Greek Olive Oil Using FT-ICR Mass Spectrometry Flow Injection Analysis and Multivariate Data Analysis**; Matthias Witt[1]; Theodora Nikou[2]; Aiko Barsch[1]; Christopher J Thompson[3]; Maria Halabalaki[2]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]University of Athens, Athens, Greece; [3]Bruker Daltonic, Billerica, MA*

ThP 494 **In-Source Ion Clustering of Bile Acids in ESI: Implications for Quantification, Instrument Operation and Non-Targeted Metabolomics Applications**; Patrick Brophy[1]; Angela Doneanu[2]; Jay Johnson[2]; Corey D Broeckling[1]; James Murphy[2]; Jessica E. Prenni[1]; *[1]Colorado State University's Proteomics and Metabolomics Facility, Fort Collins, CO; [2]Waters Corp, Milford, MA*

ThP 495 **Discovery Single-cell Mass Spectrometry Profiles Metabolic Gradients in the 16-cell Vertebrate (Frog) Embryo**; Erika P Portero[1]; Rosemary Masu Onjiko[1]; Sally A Moody[1]; Peter Nemes[1]; *[1]George Washington University, Washington , DC*

ThP 496 **Metabolic Signatures Reveal Exercise Training on Fatty Acid β-Oxidation in db/db Type 2 Diabetes Mellitus Mice**; Zongwei Cai[1]; Li Xiang[1]; *[1]Hong Kong Baptist University, Kowloon Tong, Kowloon, China*

ThP 497 **A Novel Labeled Metabolomics Workflow applying Isotope Ratio Outlier Analysis (IROA) and SWATH® Acquisition for Unambiguous Compound Identification**; Baljit Ubhi[1]; Felice de Jong[2]; Chris Beecher[2, 3]; *[1]SCIEX, Redwood City, CA; [2]IROA Technologies, Bolton, MA; [3]University of Florida, Gainesville, FL*

ThP 498 **Untargeted Metabolomic Analysis of Porcine Serum and Oral Fluid with a MLV Porcine Reproductive and Respiratory Syndrome Virus (PRRSV) Vaccine**; Aislinn A Pomfret[1]; David J Borts[1]; Jeffery J Zimmerman[1]; Yuly A Henao Diaz[1]; Luis G Giménez-Lirola[1]; Ting-Yu Cheng[1]; *[1]Iowa State University, Ames, IA*

ThP 499 **A Simplified, Integrated Solution for Untargeted Metabolomics**; Baljit Ubhi[1]; Ranjan Perera[2]; Matthew Skaley[1]; Timothy J. Garrett[3]; *[1]SCIEX, Redwood City, CA; [2]Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL; [3]University of Florida, Gainesville, FL*

ThP 500 **Metabolomic Analysis of Human Neural Stem Cells Using Nanoflow Liquid Chromatography-Tandem Mass Spectrometry**; Jingjing Deng[1]; Guoan Zhang[2]; Thomas A. Neubert[1]; *[1]New York University Langone Medical Center, New York, NY; [2]Weill Cornell Medicine, New York, NY*

ThP 501 **Metabolomics Approach to Evaluate Silver Nanoparticle Toxicity**; Samanthi I Wickramasekara[1]; Suresh Narayanasamy[1]; Steven Woolford[1]; Eric Sussman[1]; *[1]US FDA, Silver Spring, MD*

ThP 502 **Single-cell Profiling of Dorsal-Ventral Metabolomic Differences in the Vertebrate (Frog) Embryo**; David Plotnick[1]; Rosemary Masu Onjiko[1]; Peter Nemes[1]; *[1]George Washington University , Washington, DC*

ThP 503 **Metabolomic Profiling in Human Mammary Epithelial Cells (HMEC) Exposed to 1,25(OH)2D**; Renny S. Lan[1, 2]; Ping-Ching Hsu[1, 2]; Theodore M. Brasky[2]; Joseph P. McElroy[2]; Adana A. Llanos[2, 3]; Ken Riedl[2]; Steven J. Schwartz[2]; Peter G. Shields[2]; *[1]University of Arkansas for Medical Sciences, Little Rock, AR; [2]The Ohio State University, Columbus, OH; [3]Rutgers University, New Brunswick, NJ*

ThP 504 **Comparative Metabolomics of Scab Resistant and Susceptible Pecans**; Zhentian Lei[1]; David Huhman[2]; Daniel Wherritt[3]; Barbara Sumner[1]; Santosh Kumar[1]; Lloyd W. Sumner[1]; *[1]University of Missouri, Columbia, MO; [2]The Samuel Roberts Noble Foundation, Ardmore, OK; [3]University of Texas at San Antonio, San Antonio, TX*

ThP 505 **Derivatized Globally Optimized Targeted Mass Spectrometry (dGOT-MS) for Metabolomics Analysis of Carboxylic Acids**; Renke Zhang[1, 2]; Xinyu Zhang[1]; Haiwei Gu[1]; Ping Zhang[1, 3]; G. A. Nagana Gowda[1]; Liladhar Paudel[1]; Dan Du[1, 4]; Daniel Raftery[1]; *[1]Northwest Metabolomics Research Center, Department of Anesthesiology and Pain Medicine, University of Washington, Seattle, WA; [2]China Agricultural University, Haidian, China; [3]Southwest University, Beibeiqu, China; [4]West China-Washington Mitochondria and Metabolism Center, West China Hospital, Sichuan Univeristy, Chengdu, China*

ThP 506 **Comparison of High Resolution Quadrupole-Time-of-Flight and Orbitrap Mass Spectrometers for the Analysis of Small Molecules**; Marzieh Ramezani[1]; Edgar A. Arriaga[1]; *[1]University of Minnesota, Minneapolis, Minnesota*

ThP 507 **Benefits of SWATH® Acquisition, a DIA Technique over Traditional Data Dependent Analysis for High Resolution Untargeted Metabolomics Applications**; Hector Gallart-Ayala[1]; Zuzana Demianova[2]; Cyrus Papan[3]; Joerg Dojahn[2]; Baljit K. Ubhi[4]; *[1]Sciex, Alcobendas, Spain; [2]SCIEX, Darmstadt, Germany; [3]SCIEX, Darmstadt, Germany; [4]SCIEX, Redwood City, CA*

ThP 508 **Metabolic Profiling of Synthetic Cannabinoid 5F-ADB in Clinical Samples Using Non-Targeted SWATH Acquisition**; Michael Dunn[1]; Margaret Knight[1]; Clair Roper[1]; Peter Blain[1]; *[1]Medical Toxicology Centre, Newcastle University, Newcastle upon Tyne, UK*

ThP 509 **High Throughput Metabolomics of Greenhouse Grown Maize Plants Reveals Response to Drought Treatments and Predicts Field Grain Yield**; Jan Hazebroek[1]; April Agee Carroll[2]; Roland Welle[3]; Gerie van der Heijden[1]; Teresa Harp[1]; Chris Vlahakis[1]; *[1]DuPont Pioneer, Johmston, IA; [2]Purdue, West Lafayette, IN; [3]DuPont Pioneer, Eschbach, Germany*

ThP 510 **Metabolomic Profiling of Sweat Collected from Primary Lymphedema Patients Using Non-Occlusive Sample Collection and CIL LC-MS**; Kevin Hooton[1]; Ian Soles[2]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB, Canada; [2]Salutaris Centre, Edmonton, AB, Canada*

ThP 511 **Achieving Rapid Multi-Omics Analysis in Under 48 Hours**; Alexander Aksenov[1]; Robby Quinn[1]; Jose Navas-Molina[1]; Rob Knight[1]; Pieter C. Dorrestein[1]; *[1]University of California San Diego, San Diego, CA*

ThP 512 **The Development of a LC-FAIMS-MS Metabolomics Workflow: A New Tool for Untargeted Metabolite Profiling to Diagnose Disease**; Lauren Brown[1]; Kayleigh Arthur[1]; Alasdair Edge[1]; Aditya Malkar[1]; Paul Nasca[1]; *[1]Owlstone Medical Ltd., Cambridge, UK*

ThP 513 **Untargeted Metabolic Profiling of the Media of *Plasmodium falciparumisolates* Grown to Different Levels of Parasitemia**; Patricia Gonzales Hurtado[1]; Benjamin Orsburn[2]; Michal Fried[1]; *[1]Laboratory of Malaria Immunology and Vaccinology, NIAID, Rockville, Maryland; [2]Thermo Fisher Scientific, West Palm Beach, FL*

ThP 514 **Global Metabolomics Profile through the Blood-Brain Barrier of the Neurovascular Unit (NVU)**; Simona Gabriela Codreanu[1, 2]; Stacy D. Sherrod[1, 2]; Jacquelyn A. Brown[1]; Diana M. Neely[3]; BethAnn McLaughlin[3]; Aaron B. Bowman[3]; John P. Wikswo[1]; John A. McLean[1]; *[1]Vanderbilt University, Nashville, TN; [2]Center for Innovative Technology, Vanderbilt University, Nashville, TN; [3]Vanderbilt University Medical Center, Nashville, TN*

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ThP 515 **Interconversion of Protonated Imidazolidinone Ions; Isomers of [b4]+ Derived from Protonated Tetraglycine**; Brian Lam[1]; Justin Kai-Chi Lau[1, 2]; Cheuk-Kuen Lai[1, 2]; K.W. Michael Siu[1, 2]; Alan C. Hopkinson[1]; *[1]York University, Toronto, ON, Canada; [2]University of Windsor, Windsor, ON, Canada*

ThP 516 **Formation of Protonated a and b Ions from Lanthanide-Peptide Complexes**; Yating Wang[1]; Justin Kai-Chi Lau[1]; Cheuk-Kuen Lai[1, 2]; Brian Lam[1]; K.W. Michael Siu[1, 2]; Alan C. Hopkinson[1]; *[1]York University, Toronto, ON, Canada; [2]University of Windsor, Windsor, ON, Canada*

ThP 517 **Fragmentation Mechanism of Proline Containing Dipeptide**; Sabyasachy Mistry; *Purdue University, West Lafayette, IN*

ThP 518 **Fragmentation of Deprotonated Glycine and Alanine, their Di-, Tri-Peptides and Corresponding Amides Investigated by Collision-Induced Dissociation and Molecular Orbital Calculations**; Can Cui[1]; Ashley S. McNeill[2]; David A. Dixon[2]; Carolyn J. Cassady[2]; *[1]The University of Alabama, Tuscaloosa, AL; [2]The University of Alabama, Tuscaloosa, AL*

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ThP 519 **Evolution of a Mass Spectrometry-Grade PTM Directed Protease for Large Scale Post-Translational Modification Analyses**; Duc Tran[1, 2]; Valerie J Cavett[2]; Vuong Q Dang[2]; Hector L Torres[2]; Brian M Paegel[2]; *[1]Ho Chi Minh City International University, Ho Chi Minh City, Vietnam; [2]The Scripps Research Institute, Jupiter, FL*

ThP 520 **Rapid and Accurate Global PTM Discovery (G-PTM-D) Using Defined Mass Windows**; Stefan K. Solntsev[1]; Michael R. Shortreed[1]; Brian L. Frey[1]; Robert J. Millikin[1]; Anthony J. Cesnik[1]; Lloyd M. Smith[1, 2]; *[1]University of Wisconsin-Madison, Madison, WI; [2]Genome Center of Wisconsin, Madison, WI*

ThP 521 **Accurate Phosphorylation Site Localization Using Phospho-containing Site-determining Product Ions**; Zhixin Tian[1]; kaijie xiao[1]; *[1]School of Chemical Science and Engineering, Tongji University, Shanghai, China*

ThP 522 **Nontargeted Characterization of D-Amino Acid-Containing Neuropeptides**; Itamar Livnat[1]; Hua-Chia Tai[2]; Elena V. Romanova[2]; James W. Checco[2]; Jonathan V. Sweedler[2]; *[1]University of Illinois at Urbana-Champaign, Urbana, IL; [2]University of Illinois at Urbana Champaign, Urbana, IL*

ThP 523 **Characterization of L/D-Peptide Isomerase Activity in *Aplysia californica***; Hua-Chia Tai[1]; Peter M. Yau[2]; Jonathan V. Sweedler[2]; *[1]University of Illinois at Urbana-Champaign, Urbana, IL; [2]University of Illinois at Urbana-Champaign, Urbana, IL*

ThP 524 **Defining Mechanisms of Licorice Chemoprevention: Identification of Active Sites on Keap1 and Bach1 Regulating the Antioxidant Response Element**; Amanda Lee[1]; Lingyi Huang[1]; Richard B. van Breemen[1]; *[1]University of Illinois at Chicago College of Pharmacy, Chicago, IL*

ThP 525 **Characterization of tau Post-Translational Modifications in a Novel Cellular Model of tau Aggregation**; Nathan G. Hatcher[1]; Mali L. Cosden[1]; Daniel S. Spellman[1]; John M. Majercak[1]; Joel B. Schachter[1]; *[1]Merck Research Laboratories, West Point, PA*

ThP 526 **The Highly Ubiquitinated Protein Cargo of Exosomes Shed by Myeloid-Derived Suppressor Cells**; Sitara Chauhan[1]; Katherine Adams[1]; Virginia Clements[2]; Yan Wang[1]; Nathan J Edwards[3]; Suzanne Ostrand-Rosenberg[2]; Catherine Fenselau[1]; *[1]University of Maryland, College Park, MD; [2]University of Maryland Baltimore County, Baltimore, MD; [3]Georgetown University Medical Center, Washington, DC, DC*

ThP 527 **Large Scale Discovery of Post-Translational Modifications Conserved across Microbial Species**; Seungjin Na[1]; Nuno Bandeira[1]; *[1]University of California, San Diego, La Jolla, CA*

ThP 528 **Subcritical Water Processing of Proteins: Amino acid side-chain modifications**; Thomas Powell[1]; Helen J. Cooper[1]; Steve Bowra[2]; *[1]University of Birmingham, Birmingham, UK; [2]Phytatec (UK) Ltd, Plas Gogerddan, UK*

ThP 529 **Retention Time Prediction for Glycopeptides in Reversed phase Chromatography**; Evelyn Ang[1]; Vic Spicer[1]; Helene Perreault[1]; Oleg Krokhin[1]; *[1]University of Manitoba, Winnipeg, MB*

ThP 530 **Retention Time Prediction for Peptides Containing Deamidated Asn Residues in Reversed-Phase Chromatography**; Haley Neustaeter[1]; Victor Spicer[1]; Oleg Krokhin[1]; *[1]University of Manitoba, Winnipeg, MB*

ThP 531 **Controlling the False Amino-acid Rate (FAR) in De Novo Peptide Sequencing**; Hao Yang[1]; Hao Chi[1]; Wen-Feng Zeng[1]; Wen-Jing Zhou[1]; Chao Liu[1]; Si-Min He[1]; *[1]Key Lab of Intelligent Information Processing of Chinese Academy of Sciences (CAS), Beijing, China*

ThP 532 **Simple, Rapid Determination of Isobaric Amino Acids by Chemical Derivatization**; Stephen Ayrton[1]; Ryan M Bain[2]; Christopher J Pulliam[2]; Tawnya Flick[3]; R. Graham Cooks[2]; *[1], West Lafayette, IN; [2]Purdue, West Lafayette, IN; [3]Amgen, Thousand Oaks, CA*

ThP 533 **Antibody-based Target Identificationof Covalent Kinase Inhibitors and Potential Targets of Phenyl Vinyl Sulfone by Mass Spectrometry**; Chi-Chi Chou[1]; Cheng-Han Yu[2]; Geen-Dong Chang[2]; Kay-Hooi Khoo[2, 3]; *[1]Academia Sinica, Taipei; [2]National Taiwan University, Taipei, Taiwan; [3]Academia Sinica, Taipei, Taiwan*

ThP 534 **Precipitation of HPG-ALD Polymer Using Organic Solvents Improves Peptide Identification in TAILS Terminomics**; Nestor Solis[1]; Jennifer Mark[1]; Anilkumar Parambath[1]; Jayachandran Kizhakkedathu[1]; Christopher M Overall[1]; *[1]University of British Columbia, Vancouver, BC, Canada*

ThP 535 **Discovery and Identification of O-Glycosylated Signaling Peptides from Mouse and Human Pancreatic Islets Enabled by EThcD Mass Spectrometry**; Qing Yu[1]; Alejandra Canales[2]; Matthew Glover[2]; Rahul Das[2]; Xudong Shi[2]; Yang Liu[2]; Mark P Keller[2]; Alan D. Attie[2]; Lingjun Li[2]; *[1]University of Wisconsin-Madison, Madison, WI; [2]University of Wisconsin-Madison, Madison, WI*

ThP 536 **Systematic Comparison of Reduction and Alkylation Reagents reveals Side Chain Loss of Methionine due to Iodine Containing Alkylation Reagents**; Torsten Müller[1]; Dominic Winter[1]; *[1]IBMB Bonn , Bonn*

ThP 537 **Developing an Analytical Framework for Sulfoproteomics: Sulfopeptide Enrichment and Positive Mode Mass Spectrometric Analysis**; Hye Kyong Kweon[1]; Brian L. Tang[1]; Phillip J. McClory[1]; Philip C. Andrews[1]; Kristina Hakansson[1]; *[1]University of Michigan, Ann Arbor, MI*

ThP 538 **Data-Independent Infrared Multi-Photon Dissociation for the Targeted Discovery of Cysteine Sulfonic Acid**; Nicholas B. Borotto[1]; Phillip J. McClory[2]; Brent R. Martin[2]; Kristina Hakansson[2]; *[1]University of Michigan, Ann Arbor, MI; [2]University of Michigan, Ann Arbor, Michigan*

ThP 539 **HILIC LC/MS Analytical Approach for Identification of Protein Deamidation and Isomerization Modifications**; Barry Boyes[1, 2]; Majors Badgett[2]; Ron Orlando[2]; *[1]Advanced Materials Technology Inc,, Wilmington, DE; [2]Complex Carbohydrate Research Center, University of Georgia, Athens, GA*

ThP 540 **Evaluation of Methods for Selective Isolation of Cysteine-Containing Peptides in Redox-Proteomics**; Muhammad Tahir[1]; Honggang Huang[1]; Martin R. Larsen[1]; *[1]Univ. Southern Denmark, Odense*

ThP 541 **Mass Spectrometry Analysis of Sulfonation Cysteines in Peroxiredoxin 1**; Changgong Wu; *Center for Advanced Proteomics Research and the Department of Microbiology, Biochemistry and Molecular Genetics, Rutgers University, Newark, NJ*

ThP 542 **Optimization of SimSpectraST Search Conditions for Phosphoproteomics**; Tomoya Tsubosaka[1]; Ayano Takai[1]; Satoko Akahori[1]; Seiya Kawahara[1]; Veronika Suni[2]; Susumu Y. Imanishi[1]; *[1]Meijo University, Nagoya, Aichi; [2]University of Turku, Turku, Finland*

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ThP 543 **Multiplex Quantitation of Crustacean Neuropeptides after Hypoxia Exposure Using Custom 4-plex Dimethylated Leucine (DiLeu) Isobaric Tags**; Chris Sauer[1]; Amanda Buchberger[1]; Kellen DeLaney[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

ThP 544 **Multifaceted Quantitation and Imaging of Changes in Crustacean Neuropeptidome Resulting from Food Intake**; Kellen DeLaney[1]; Lingjun Li[1, 2]; *[1]University of Wisconsin - Madison Department of Chemistry, Madison, WI; [2]University of Wisconsin-Madison School of Pharmacy, Madison, WI*

ThP 545 **Induced Expression of Bioactive Peptides in *Solanum lycopersicum* under Salt Stress Conditions**; Tessa E. Bartges[1]; Christine L. Kirkpatrick[1]; Nazia Kanwal[2]; Amer Jamil[2]; Leslie M. Hicks[1]; *[1]Department of Chemistry, University of North Carolina at Chapel Hil, Chapel Hill, NC; [2]Department of Biochemistry and Molecular Biology, University of Agriculture Faisalabad, Faisalabad, Pakistan*

ThP 546 **Functional Discovery of Neuropeptides in Blue Crab, *Callinectes sapidus*, in Response to Ocean Acidification**; Yang Liu[1]; Amanda Buchberger[1]; Kellen DeLaney[1]; Lingjun Li[1, 2]; *[1]University of Wisconsin - Madison Department of Chemistry, Madison, WI; [2]University of Wisconsin-Madison School of Pharmacy, Madison, WI*

ThP 547 **Profiling Peptidomic Changes in Major Brain Regions in Response to Cocaine Intoxication and Withdrawal**; Fengfei Ma[1]; Pingli Wei[2]; Jingxin Wang[3]; Vaishali Bakshi[3]; Brian Baldo[3]; Lingjun Li[1, 2]; *[1]University of Wisconsin-Madison School of Pharmacy, Madison, WI; [2]University of Wisconsin - Madison Department of Chemistry, Madison, WI; [3]University of Wisconsin-Madison, Madison, WI*

ThP 548 **Differential Quantification of Ageing and Dehydration Effects on Peptide Secretion in the Pituitary by Automated MALDI-TOF MS**; Elena Romanova[1]; Michael P. Greenwood[2]; Mingkwan Greenwood[2]; David Murphy[2]; Jonathan V Sweedler[3]; *[1]University of Illinois at Urbana-Champaign, Urbana, IL; [2]University of Bristol, Bristol, UK; [3]University of Illinois at Urbana Champaign, Urbana, IL*

ThP 549 **Multifaceted Mass Spectrometric Analyses of Feeding-related Metabolomic and Peptidomic Changes in the Rock Crab, *Cancer irroratus***; Qinjingwen Cao[1]; Qing Yu[2]; Bingming Chen[2]; Chuanzi OuYang[1]; Fengfei Ma[2]; Lingjun Li[1, 2]; *[1]Department of chemistry, University of Wisconsin Madison, Madison, WI; [2]School of pharmacy, University of Wisconsin Madison, Madison, WI*

ThP 550 **Peptidogenomic Capture of Microprotein Virulence Factors in Community-Associated *Staphylococcus aureus***; Jacob Wozniak[1]; John Lapek[1]; Julieta Aguilar[1]; Dominic McGrosso[1]; David Gonzalez[1]; Michael Dores[2]; Ross Corriden[1]; Anvesh Marchela[1]; JoAnn Trejo[1]; Eri Nakatani-Webster[3]; Abhinav Nath[3]; Brian Werth[3]; *[1]UCSD, La Jolla, CA; [2]Hofstra Northwell School of Medicine, Hempstead, NY; [3]University of Washington, Seattle, WA*

ThP 551 **Top-down and Bottom-up Proteomics for the Identification of Crustacean Neuropeptides and Precursor-Related Peptides Predicted by Transcriptomics**; Cindy Rivera[1]; Julia M. Michels[1]; Caroline Q. Corban[1]; Patsy S. Dickinson[1]; Andrew E. Christie[2]; Elizabeth A. Stemmler[1]; *[1]Bowdoin College, Brunswick , ME; [2]University of Hawaii at Manoa, Honolulu, Hawaii*

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ThP 552 **Proteomics and Phospho-Proteomics of Fertilization: Immature Oocyte to Late Neurula Stage Embryo**; Elizabeth Peuchen[1]; Liangliang Sun[2]; Olivia F Cox[1]; Alex Hebert[3]; Joshua Coon[3]; Mathew F Champion[1]; Paul W Huber[1]; Norman J Dovichi[1]; *[1]University of Notre Dame, Notre Dame, IN; [2]Michigan State University, Lansing, MI; [3]University of Wisconsin-Madison, Madison, WI*

ThP 553 **Time-Resolved Quantitative Analysis of Cellular Signaling and Epigenetic Mechanisms During Epithelial-Mesenchymal Transition**; Congcong Lu[1]; Simone Sidoli[1]; Zuofei Yuan[1]; Benjamin A. Garcia[1]; *[1]University of Pennsylvania, Philadelphia, PA*

ThP 554 **Accumulated Ion Monitoring (AIM) Enables Enrichment-Free Quantitation of Rare and Phosphorylated Peptides from Micrograms and Thousands of Human Cells**; Paolo Cifani[1]; Alex Kentsis[1, 2]; *[1]Molecular Pharmacology Program, Sloan Kettering Institute, Memorial Sloan Kettering Cancer Center, New York, NY; [2]Department of Pediatrics, Weill Medical College of Cornell University and Memorial Sloan Kettering Cancer Center, New York, NY*

ThP 555 **Dephosphorylation of AMA1 Cytosolic Tail during *Toxoplasma gondii* Invasion**; Shruthi Krishnamurthy[1]; Bin Deng[1]; Roxana del Rio[1]; Kerry R. Buchholz[2]; Moritz Treeck[2]; Siniša Urban[3]; John Boothroyd[2]; Ying Wai Lam[1]; Gary E. Ward[1]; *[1]University of Vermont, Burlington, VT; [2]Stanford School of Medicine, Stanford, CA; [3]Johns Hopkins University School of Medicine, Baltimore, MD*

ThP 556 **A Phosphoproteomic Approach to Investigate Mechanical Sensing in *Xenopus laevis* Embryos**; Yutaka Hashimoto[1, 2]; Noriyuki Kinoshita[2]; Todd M. Greco[1]; Pierre Jean Beltran[1]; Joel Federspiel[1]; Naoto Ueno[2]; Ileana M. Cristea[1]; *[1]Princeton University, Princeton, NJ; [2]National Institute for Basic Biology, Okazaki, Japan*

ThP 557 **Identification of Potential Mitotic CK2 Substrates and Interactors by Quantitative Phosphoproteomics**; Scott Rusin[1]; Arminja N Kettenbach[1, 2]; *[1]Dartmouth College, Hanover, NH; [2]Norris Cotton Cancer Center, Lebanon, NH*

ThP 558 **Nano LC-MS Based Phosphoproteomic Approach for Evaluating Signaling Properties of Insulin Receptor Agonists**; Zhongping Liao[1]; Jason X. Tang[2]; *[1]Eli Lilly and Company, Indianapolis, IN; [2]Eli Lilly and Company, Indianapolis, IN*

ThP 559 **Quantitative Chemical Phosphoproteomics Identifies PCTAIRE-1 (Cdk16) as a Novel Wee1 Substrate**; Andrew Grassetti[1]; Rufus Hards[2]; Scott A Gerber[2]; *[1], Lebanon, NH; [2]Dartmouth College, Hanover, NH*

ThP 560 **Kinase Activity Profiling by Motif-Targeting Phosphoproteome Analysis**; Chia-Feng Tsai[1]; Masaki Wakabayashi[1]; Naoyuki Sugiyama[1]; Yasushi Ishihama[1]; *[1]Graduate School of Pharmaceutical Sciences,Kyoto University, Kyoto City, Japan*

ThP 561 **Benchmarking LFQ, SILAC and MS2/MS3-based TMT Quantification Strategies for Phosphoproteomics**; Alexander Hogrebe[1]; Louise von Stechow[1]; Dorte B. Bekker-Jensen[1]; Brian T. Weinert[1]; Christian D. Kelstrup[1]; Jesper V. Olsen[1]; *[1]The Novo Nordisk Foundation Center for Protein Research, Proteomics Program, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark*

ThP 562 **Multiplexing Meets Automation: TMT-Labeling in PRM Assays Increases Sample Throughput and Allows for Precise Relative Quantification**; Malvina Papanastasiou[1]; Alvaro Sebastian Vaca Jacome[1]; Adam Officer[1]; Katherine DeRuff[1]; Steven A. Carr[1]; Jacob D. Jaffe[1]; *[1]Broad Institute of MIT and Harvard, Cambridge, Massachusetts*

ThP 563 **Identification of physiological kinase substrates from cell extracts by differential phosphorylation using reverse in-gel kinase assay and nano-LC tandem MS**; Weiliang Huang[1]; Xiang Li[2]; Keqi Tang[3]; Maureen A. Kane[1]; Charles J. Bieberich[2]; *[1]University of Maryland, School of Pharmacy, Department of Pharmaceutical Sciences, Baltimore, MD; [2]University of Maryland Baltimore County, Department of Biological Sciences, Baltimore, MD; [3]Pacific Northwest National Laboratory, Biological Sciences Division, Richland, WA*

ThP 564 **Establishing the Basal Global Phosphorylation Stoichiometry of a Human Colorectal Carcinoma Cell Line Using TMT-Based Multiplexed Proteomics**; Matthew Y. Lim[1]; Joao A. Paulo[1]; Steven P. Gygi[1]; *[1]Harvard Medical School, Boston, MA*

ThP 565 **Quantitative Phosphoproteomic Analysis of Circadian Clock-Associated Kinases in *Arabidopsis thaliana***; Shin-Cheng Tzeng[1]; Margret Wilson[1]; Matthew Meyer[1]; Xiaoyue Jiang[2]; Jae Choi[3]; John Bulter[2]; Dmitri Nusinow[1]; Bradley Evans[1]; *[1]Donald Danforth Plant Science Center, St. Louis, MO; [2]Thermo Fisher Scientific, San Jose, California; [3]Thermo Fisher Scientific, Rockford, IL*

ThP 566 **Quantitative Phosphoproteomics Unveils Novel phosphorylation Events in Transformed Human Bronchial Epithelial Cell Induced by Arsenic**; Yue Qi[1]; Lingzhi Li[1]; Michael Caruso[1]; Xiangmin Zhang[1]; Fei Chen[1]; Zhengping Yi[1]; *[1]Wayne State University, Detroit, Michigan*

ThP 567 **Going Deep: A Comprehensive Analysis of Tissue-Specific Protein Phosphorylation and Expression**; Katie J Clowers[1]; Mark P Jedrychowski[1]; Edward L Huttlin[1]; John Szpyt[1]; Joao A Paulo[1]; Steven P Gygi[1]; *[1]Harvard Medical School, Boston, MA*

ThP 568 **The Phosphoproteome as a Phenotype: Towards a high throughput Platform for Phosphoproteomics**; Matthew Foley[1, 2]; Michael J. Ford[2]; Richard C. Jones[2]; Ravi Amunugama[2]; David L. Allen[2]; *[1]University of Michigan, Ann Arbor, Michigan; [2]MS Bioworks, Ann Arbor, MI*

ThP 569 **High-Resolution Phosphoproteomic Identification of Zika Virus-Initiated Events in Host Cells**; Ronik Khachatoorian[1]; Whitaker Cohn[2]; Austin Quach[2]; James Vu[1]; Natalie Liu[1]; Nu Lu[1]; Travis Moller[2]; Piotr Ruchala[2]; Vaithilingaraja Arumugaswami[3]; Samuel French[1]; Julian Whitelegge[2]; *[1]Department of Pathology and Laboratory Medicine, David Geffen School of Medicine at University of California, Los Angeles, CA; [2]Pasarow Mass Spectrometry Laboratory and Neuropsychiatric Institute–Semel Institute for Neuroscience & Human Behavior, David Geffen School of Medicine at UCLA, Los Angeles, California; [3]Department of Surgery, The Board of Governors Regenerative Medicine Institute at Cedars-Sinai Medical Center, Los Angeles, CA*

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ThP 570 **Prediction of Deamidation Rates of Proteins to Assess their Long-Term Stability Using Hydrogen Exchange Mass Spectrometry (HX-MS)**; Chamalee L D Gamage[1]; David D Weis[1, 2]; *[1]Department of Chemistry, University of Kansas, Lawrence, KS; [2]Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS*

ThP 571 **Site-Specific Characterization of PEGylated Insulin Isomers by Using Combined Liquid Chromatography and Ion Mobility Mass Spectrometry**; Selim Gerislioglu[1]; Scott Adams[1]; Chrys Wesdemiotis[1]; *[1]The University of Akron, Akron, OH*

ThP 572 **Applications of Native Mass Spectrometry (MS) for Biotherapeutics Characterization and Associated Challenges**; Olga Friese[1]; Thomas W. Powers[1]; Jacqyelynn Smith[1]; Paul Brown[1]; Andrew Dawdy[1]; Jason C. Rouse[2]; *[1]Pfizer, Inc., St. Louis, MO; [2]Pfizer, Inc., Andover, MA*

ThP 573 **Discovery, Characterization, and Remediation of an Fc-extension in Proteins Expressed in CHO Cells**; Stone D.-H. Shi[1]; Christopher S. Spahr[1]; Mark E. Daris[1]; Kevin C. Graham[1]; Brian D. Soriano[1]; Jennitte L. Stevens[1]; *[1]Amgen, Thousand Oaks, CA*

ThP 574 **Orthogonal Mass Spectrometry-Based Footprinting Strategies Characterize the Epitope and a Structural Rearrangement of Interleukin-6 Receptor Subunit Alpha upon Adnectin Binding**; Ke Sherry Li[1]; Guodong Chen[2]; Jingjie Mo[2]; Richard Y-C Huang[2]; Ekaterina Deyanova[2]; Brett Beno[2]; Steve O'neil[2]; Adrienne A. Tymiak[2]; Michael L. Gross[3]; *[1]Washington University, St. Louis, MO; [2]Bristol-Myers Squibb, Princeton, NJ; [3]Washington University, St Louis, MO*

ThP 575 **Mapping of Complex Disulfide Patterns with Closely-Spaced Cysteines by In-Source Reduction and Data-Dependent Mass Spectrometry**; Christian Cramer[1, 2]; Christian D. Kelstrup[2]; Jesper V. Olsen[2]; Kim F. Haselmann[1]; Peter Kresten Nielsen[1]; *[1]Novo Nordisk A/S, Maaloev, DK; [2]CPR - Center for Protein Research, Copenhagen, Denmark*

ThP 576 **Development of a Fast Proteinase K Digestion Protocol for Characterization of Fluorescein Isothiocyanate Labeled Recombinant Human Insulin**; Fanyu Meng[1]; Ross Yang[1]; Weijuan Tang[1]; Li-Kang Zhang[1]; Bing Mao[1]; *[1]Merck & Co., Inc, Rahway, NJ*

ThP 577 **Automated Determination of Induced Monoclonal Antibody Disulfide Bond Shuffling Using Multiple Enzyme Digestions**; Christopher A Bolcato[1]; Katy Ryan[1]; Heather Anderson[1]; Matthew J Powell[1]; K. Ilker Sen[2]; St. John Skilton[2]; Eric Carlson[3]; Matthew D Maust[1]; *[1]Protea Biosciences, Morgantown, WV; [2]Protein Metrics, San Carlos, CA; [3]Protein Metrics Inc., San Carlos, CA*

ThP 578 **Characterization of a Novel Modification of a CHO Produced mAb: Evidence for the Presence of Tyrosine Sulfation**; Jia Zhao; *Merck, Kenilworth , NJ*

ThP 579 **Optimizing Biotherapeutics Size-based Characterization by Native Mass Spectrometry**; Leah (Hanliu) Wang[1]; Thomas W. Powers[1]; Ying Zhang[2]; Cliff Entrican[2]; Jacquelynn Smith[1]; Andrew W. Dawdy[1]; Yin Luo[2]; Jason C. Rouse[2]; OLGA FRIESE[1]; *[1]Biotherapeutics Pharm. Sci., Pfizer Inc., St. Louis, MO; [2]Biotherapeutics Pharm. Sci., Pfizer Inc., Andover, MA*

ThP 580 **Subtle Structural Changes to Antibody Therapeutics Detected Using Diethylpyrocarbonate Labeling and Mass Spectrometry**; Patanachai (Kong) Limpikirati[1]; John E. Hale[2]; Eric M. Graban[2]; Robert C. Vaughan[3]; Richard W. Vachet[1]; *[1]Department of Chemistry, University of Massachusetts Amherst, Amherst, MA; [2]QuarryBio, Bloomington, IN; [3]Department of Molecular and Cellular Biochemistry, Indiana University, Bloomington, IN*

ThP 581 **Study of Stressed Monoclonal Antibody (mAb) Pharmaceuticals by Using Deep-UV Resonance Raman (DUVRR) Spectroscopy and MALDI-TOF Mass Spectrometry**; Chen Qiu[1]; Jamie Mans[1]; Sergey Arzhantsev[1]; *[1]US FDA, St. Louis, MO*

ThP 582 **Tyrosine to Phenylalanine Sequence Variants Observed During Cell Line Development for Manufacture of a Monoclonal Antibody**; Thomas Slaney[1]; Mina Chaudhry[1]; Hangtian Song[1]; Wei Wu[1]; Li Tao[1]; Tapan Das[1]; *[1]Bristol-Myers Squibb, Hopewell, NJ - New Jersey*

ThP 583 **Dialysis-Coupled Hydrogen/Deuterium Exchange Mass Spectrometry Allows Conformational Analysis of Therapeutic Monoclonal Antibodies at Extreme Concentrations**; Zeinab Nazari[1, 2]; Damian Houde[3]; Marco van de Weert[1]; George Bou-Assaf[2]; Andrew Weiskopf[2]; Kasper Dyrberg Rand[1]; *[1]Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; [2]Department of Protein Pharmaceutical Development, Biogen, Cambridge, MA; [3]Codiak BioSciences, Cambidge, MA*

ThP 584 **Data Independent Top-Down Characterization of Proteins for Biotherapeutic Applications**; Lindsay Morrison[1]; Brad Williams[1]; *[1]Waters Corporation, Beverly, MA*

ThP 585 **Detection and Characterization of N- and O-Glycosylation: Streamlined Methods for Intact Mass Analysis and Bottom-Up Proteomics**; Paula Magnelli[1]; Colleen McClung[1]; Cristian Ruse[1]; Ellen Guthrie[1]; Stephen Shi[1]; *[1]New England BioLabs, Ipswich, MA*

ThP 586 **Impact of Tryptophan Oxidation in Complementarity-Determining Regions on Structure-Function Characterized by Hydrogen Exchange Mass Spectrometry and Surface Plasmon Resonance**; Tyler

Hageman[1, 2]; Hui Wei[2]; Patrick Kuehne[2]; Jinmei Fu[2]; Richard Ludwig[2]; Li Tao[2]; Tapan Das[2]; *[1]University of Kansas, Lawrence, KS; [2]Bristol-Myers Squibb, Pennington, NJ*

ThP 587 **Direct Mass Spectrometric Characterization of Disulfide Linkages**; Xiaoyan Guan[1]; Le Zhang[1]; Jette Wypych[1]; *[1]Amgen Inc., Thousand Oaks, CA*

ThP 588 **Toward Chemical Footprinting at Residue Resolution: FPOP Data Analysis of IL23 - Antibody Binding**; Jing Li[1]; Ke Li[1]; Michael L. Gross[1]; Ekaterina Deyanova[2]; Richard Huang[2]; Yun Wang[2]; Robert Langish[2]; Adrienne A. Tymiak[2]; Guodong Chen[2]; Kadir Ilker Sen[3]; Eric Carlson[3]; Christopher Becker[3]; *[1]Washington University, St Louis, MO; [2]Bristol-Myers Squibb, Princeton, NJ; [3]Protein Metrics Inc., San Carlos, CA*

ThP 589 **Capillary Electrophoresis - Mass Spectrometry (IP-CE-MS) Analysis of Protein Therapeutics for Identification of *in vivo* Catabolites** ; Mei Han[1]; Josh T. Pearson[1]; Yunan Wang[1]; Dan A. Rock[1]; Brooke M. Rock[1]; *[1]Amgen, South San Francisco, CA*

ThP 590 **Sample Preparation Method for Accurate Analysis of Non-Enzymatic PTMs in Biotherapeutic Proteins with Peptide Mapping**; Sergei Saveliev[1]; Chris Hosfield[1]; Michael Rosenblatt[1]; Marjeta Urh[1]; *[1]Promega Corporation, Madison, WI*

ThP 591 **Protein Disulfide Bond Characterization with DMS and ECD**; J.C. Yves Leblanc[1]; Brendon Seale[1, 2]; Lyle Burton[1]; Takashi Baba[1]; *[1]SCIEX, Concord, ON, Canada, ON, Canada; [2]University of Toronto, Toronto, ON, Canada*

ThP 592 **Improvement of Glycosylation Profile to Increase Similarity of Adalimumab Biosimilar to the Innovator with High-Resolution Mass Spectrometry**; Ahmet Emin Atik[1]; Zeynep Yildirim Keles[1]; Yigit Erdemgil[1]; Deniz Baycin Hizal[1]; Ozge Can[2]; R. Serdar Alpan[1]; *[1]Turgut Ilaclari Biotechnology Group, İstanbul, Turkey; [2]Department of Medical Engineering, Acibadem University, İstanbul, Turkey*

ThP 593 **Characterizing Monoclonal Antibody (mAb) Epitopes and Paratopes Using Structural Mass Spectrometry**; Janna Kiselar[1, 2]; John Schenkel[3]; Mark Chance[2, 4]; *[1]Case Western Reserve University, Cleveland, OH; [2]Department of Nutrition, Case Western Reserve University, Cleveland, OH; [3]NeoProtoemics, Inc., Cleveland, OH; [4]Case Western Reserve University, Cleveland, OH*

ThP 594 **Systematic Analysis of the Truncations and Modifications of Bovine Pulmonary Surfactant Proteins B and C in Natural Alternative Medicine**; Lian Shu[1]; Jifeng Wang[1]; Zhengsheng Xie[1]; Lili Niu[1]; Xiang Ding[1]; Xiaojing Guo[1]; Tanxi Cai[1]; Fuquan Yang[2]; *[1]Institute of Biophysics, Chinese Academy of Sciences, Beijing, China; [2]Institute of Biophysics, CAS, Beijing, Beijing*

ThP 595 **An Improved Workflow for Sequence Confirmation and PTM Identification of Monoclonal Antibodies Using Middle-Down ETD and CID Fragmentation**; Weibin Chen[1]; Henry Shion[1]; Nilini Ranbaduge[1]; Francesco Lanucara[2]; Emmy Hoyes[2]; Jeff Brown[2]; Jonathan P Williams[2]; James Langridge[2]; *[1]Waters Corp, Milford, MA; [2]Waters Corp., Wilmslow, UK*

ThP 596 **A Multi-level Quantitative Estimation of mAb Clipping**; Harsha Gunawardena[1]; Eric Beil[1]; Andy Mahan[1]; Jeff Brelsford[1]; Hirsh Nanda[1]; *[1]Janssen R&D of Johnson & Johnson, Greater Philadelphia, PA*

ThP 597 **Comprehensive Characterization of the NIST mAb Reference Standard Using an IMS QTof Mass Spectrometer**; Nilini Ranbaduge[1]; Jing Fang[2]; William Alley[2]; Henry Shion[2]; Ying Qing Yu[2]; *[1]Waters Corporation, Milford, Massachusetts; [2]Waters Corp, Milford, MA*

ThP 598 **Native Ion Exchange Chromatography Orbitrap Mass Spectrometry Allows Surface Charge Discrimination and Online Detection of Intact Proteins for Deep Characterization**; Aaron O. Bailey[1]; Guanghui Han[2]; Wendy Sandoval[2]; Jonathan L. Josephs[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Genentech, Inc, South San Francisco, CA*

ThP 599 **A General Optimized Protocol for Sequence and Glycoforms Characterization of Monoclonal Antibodies**; Modupeola A Sowole[1]; Lin He[2]; Baozhen Shan[2]; Gilles A. Lajoie[3]; *[1]University of Western Ontario, London, ON, Canada; [2]Bioinformatics Solutions Inc, Waterloo, ON, Canada; [3]University of Western Ontario, London , ON, Canada*

ThP 600 **Development of LC-MS Platform Methods for IgG Analysis Using Q-Exactive Plus**; Alisa Marie VanGrunsven[1]; Emilie Aude Viglino[1]; *[1]CMC Biologics, Bothell, Washington*

ThP 601 **High Efficiency Wide Pore Superficially Porous Particles for LC/MS of Larger Proteins**; Stephanie A. Schuster[1]; Brian M. Wagner[1]; Benjamin P. Libert[1]; William L. Miles[1]; Barry E. Boyes[1, 2]; *[1]Advanced Materials Technology, Inc., Wilmington, DE; [2]Complex Carbohydrate Research Center, University of Georgia, Athens, GA*

ThP 602 **Automated Intact Mass Analysis for the Characterization of Antibodies**; Maurizio Bronzetti[1]; Joe Shambaugh[1]; David Bush[1]; Stefano Gotta[2]; Cassandra Wigmore[2]; Arnd Brandenburg[2]; *[1]Genedata Inc, Lexington, MA; [2]Genedata AG, Basel, Switzerland*

ThP 603 **Higher Order Structure of Intact Proteins by Capillary Electrophoresis Native Ion Mobility Mass Spectrometry**; Caroline S. Chu[1]; Pat D. Perkins[2]; Andy Gieschen[3]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]Agilent Technologies Inc., Santa Clara, CA; [3]Agilent Technologies Inc., La Jolla, CA*

ThP 604 **Simple and Quick MS Analysis of Chemically Synthesized Glycopeptides: Hydrogen/Deuterium Exchange (HDX)/MS for Verifying Racemization**; Izumi Sakamoto[1]; Kenji Hirose[2]; *[1]AcroScale Inc., Sendai, Japan; [2]Nihon Waters K.K., Osaka, Japan*

ThP 605 **Pulsed HDX-MS Probes Protein Aggregate Intermediates – Preliminary Study of GCSF Aggregation**; Jun Zhang[1]; Michael J. Treuheit[1]; *[1]Amgen, Inc, Thousand Oaks, CA*

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ThP 606 **Characterization of Protein Recognition Motifs within Heparin Chains: Online Size Exclusion Chromatography-Mass Spectrometry Based Solution Phase Footprinting**; Chendi Niu[1]; Yunlong Zhao[1]; Igor A. Kaltashov[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

ThP 607 **Studying Protein-Protein Complexes by Gas-Phase hydrogen/Deuterium Exchange Mass Spectrometry (Gas-Phase HDX-MS)**; Ulrik Hvid Mistarz[1]; Shane A Chandler[2]; Justin L P Benesch[2]; Kasper D Rand[1]; *[1]Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; [2]Department of Chemistry, University of Oxford, Oxford, UK*

ThP 608 **Gas Phase Activation Energies of Protein-Protein Interactions Determined by Electrospray Mass Spectrometry**; Yelena Yefremova[1]; Teresa F.I. Melder[1]; Bright D. Danquah[1]; Kwabena F.M. Opuni[1]; Cornelia Koy[1]; Knut Koelbel[2]; Frank Sobott[2]; Harald Illges[3]; Michael O. Glocker [1]; *[1]Proteome Center Rostock, Rostock , Germany; [2]University of Antwerp, Antwerp, Belgium; [3]University of Applied Sciences Bonn-Rhein-Sieg, Bonn, Germany*

ThP 609 **Engineering Nanodiscs for Membrane Protein Native Mass Spectrometry**; Michael Thomas Marty; *University of Arizona, Tucson, AZ*

ThP 610 **Binding Affinity and Kinetics of Transient Protein-Protein Interactions by SEC/MS Measurements**; Honglin Yao[1]; Muneeruddin Khaja[1]; Andrei N. Lipatnikov[2]; Cedric E. Bobst[1]; Igor A. Kaltashov[1]; *[1]University of Massachusetts-*

Amherst, Amherst, MA; [2]Chalmers University of Technology, Gothenburg, Sweden

ThP 611 **Quantifying Non-Covalent Complexes of Insulin with Ca(II), Mg(II), Na(I) and K(I) Electrolyte Ions by Using ESI-MS Method**; Mustafa Gulfen[1]; Abdil Ozdemir[2]; Jung-Lee Lin[3]; Chung-Hsuan Chen[3]; *[1], Adapazarı, Sakarya; [2]Sakarya University , Adapazari, Sakarya; [3]Academia Sinica, Taipei, Taiwan*

ThP 612 **Optimization of Proteomic Profiling Approaches for the Cellular Thermal Shift Assay (CETSA) Using Glucosylceramidase-Isofagomine (GBA-IFG) as a Model System**; Clifford Phaneuf[1]; PAUL Mason[1]; Alexander R. Ivanov[2]; David Bush[3]; Alexei Belenky[1]; *[1]Genzyme, Waltham, ma; [2]Northeastern University, Boston, MA; [3]Genedata, Lexington, MA*

ThP 613 **Development of Surface Induced Dissociation on a High Mass Range Orbitrap Platform with Applications Toward the Study of Protein Complexes**; Zachary L. VanAernum[1]; Joshua D. Gilbert[1]; Mikhail E. Belov[2]; Alexander A. Makarov[2]; Stevan R. Horning[2]; Vicki H. Wysocki[1]; *[1]The Ohio State University, Columbus, OH; [2]Thermo Fisher Scientific, 28199, Germany*

ThP 614 **A Rapid Mixing Device to Detect Early Intermediates in Hepatitis B Virus Assembly by Charge Detection Mass Spectrometry**; Nicholas Lyktey[1]; Corinne Lutomski[1]; Zhongchao Zhao[1]; Adam Zlotnick[1]; Martin Jarrold[1]; *[1]Indiana University, Bloomington, IN*

ThP 615 **Impact of Charge State on Dissociation of Multimeric Protein Complexes**; Sarah Sipe[1]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

ThP 616 **Enhanced Detection of Non-Covalently Bound Enzyme Complexes Using a Dedicated Large Molecule Autotune on a Q-TOF Mass Spectrometer**; Christian Klein[1]; Huy Bui[1]; Alex Mordehai[1]; Caroline S. Chu[1]; Gregor Overney[1]; William E. Barry[1]; *[1]Agilent Technologies, Santa Clara, CA*

ThP 617 **Charge State and Stoichiometry Determination for Extremely Congested Mass Spectra of Single- and Mixed-Lipid Membrane Models Using Fourier Analysis**; James S. Prell[1, 2]; Sean P. Cleary[1]; *[1]Department of Chemistry and Biochemistry, University of Oregon, Eugene, OR; [2]Materials Science Institute, University of Oregon, Eugene, OR*

ThP 618 **Untargeted Characterization of Protein Complex Stoichiometry and Cofactor Binding with Native Proteomics**; Owen Skinner[1]; Nicole A Haverland[1]; Luca Fornelli[1]; Rafael D Melani[1]; Luis H. F. Do Vale[1, 2]; Henrique S Seckler[1]; Peter F Doubleday[1]; Luis F Schachner[1]; Kristina Srzentić[1]; Neil L Kelleher[1]; Philip D Compton[1]; *[1]Northwestern University, Evanston, IL; [2]University of Brasilia, Brasilia, Brazil*

ThP 619 **Functional Analysis of Soluble and Membrane-Associated Protein Complexes by Multi-Dimensional Protein Correlation Profiling**; Zach McBride[1]; Donglai Chen[2]; Jun Xie[2]; Daniel Szymanski[2]; *[1]Purdue University, West Lafayette, IN; [2]Purdue University, West lafayette, Indiana*

ThP 620 **LC-MS Compatible Sample Preparation Using On-bead Digestion to Characterize Protein-Protein Interactions in Early Mouse Embryonic Cortical Development**; Philip Loziuk[1]; Caroline Johnson[2]; Troy Ghashghaei[2]; *[1]North Carolina State University , Raleigh, NC; [2]North Carolina State University, Raleigh, NC*

ThP 621 **A Modified flow-FPOP Platform for Oxidative Footprinting of Size-Fractionated Complexes**; Manolo D. Plasencia[1]; Don L. Rempel[2]; Michael L. Gross[2]; *[1]University of Michigan, Ann Arbor, MI; [2]Washington University, St. Louis, MO*

ThP 622 **Native LESA Mass Spectrometry: Direct Analysis of Proteins and their Complexes**; Rian L. Griffiths[1]; Victor A. Mikhailov[2]; Emma K. Sisley[1]; Helen J. Cooper[1]; *[1]University of Birmingham, Birmingham, UK; [2]University of Oxford, Oxford, UK*

ThP 623 **Native Mass Spectrometry Measurements Directly from Crude Cell Lysates**; Jinrui Gan[1]; Gili Ben-Nissan[1]; Galina Arkind[1]; Mark Tarnavsky[1]; Devin Trudeau[1]; Lianet Noda Garcia[1]; Dan S. Tawfik[1]; Michal Sharon[1]; *[1]Weizmann Institute of Science, Rehovot, Rehovot*

ThP 624 **Deconvolving Extremely Congested Mass Spectra of Nanodisc Membrane Models and Polymers Using Overtone Data from Fourier Transformed Spectra**; Sean P. Cleary[1]; James S. Prell[1, 2]; *[1]Department of Chemistry and Biochemistry, University of Oregon, Eugene, OR; [2]Materials Science Institute, University of Oregon, Eugene, OR*

ThP 625 **Cryogenic Ion Mobility-Mass Spectrometry Directly Observes Dimer Dehydration of Insulin**; Michael J. Hebert[1]; David H Russell[1]; *[1]Texas A&M University, College Station, TX*

ThP 626 **Evaluation for the Need of Adequate Sample Size for Affinity Purification-Mass Spectrometry**; Pamela S. Cantrell[1]; Mai Sun[1]; Nathan A. Yates[1, 2]; Xuemei Zeng[1]; *[1]Biomedical Mass Spectrometry Center, University of Pittsburgh Health Sciences Core Research Facilities, Pittsburgh, PA; [2]University of Pittsburgh School of Medicine, Pittsburgh, PA*

ThP 627 **Combining Native Mass Spectrometry with Mechanistic Binding Models to Define Microscopic Thermodynamics of Homotropic Allostery in Oligomeric Proteins**; Melody Holmquist[1]; Bryant Jacob[1]; Eilhu C. Ihms[1]; Paul Gollnick[2]; Vicki H. Wysocki[1]; Mark P. Foster[1]; *[1]The Ohio State University, Columbus, OH; [2]University at Buffalo, Buffalo, NY*

ThP 628 **Developing LC-MS Methods to Characterize the Interaction of Therapeutic Proteins with Heparin Oligosaccharides**; Cedric E. Bobst[1]; Igor A. Kaltashov[2]; *[1]University of Massachusetts, Amherst, MA; [2]University of Massachusetts Amherst, Amherst, MA*

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ThP 629 **Cytochrome c as a Peroxidase: Covalent Labeling and Oxidation Site Mapping Uncovers the Mechanism of Catalytic Activation by H2O2**; Victor Yin[1]; Gary S Shaw[1]; Lars Konermann[1]; *[1]University of Western Ontario, London, ON, Canada*

ThP 630 **Quantitative Crosslinking and Quantitative Surface Modification for the Structural Characterization of Disorder-To-Order Transitions**; Karl A.T. Makepeace[1]; Evgeniy V. Petrotchenko[2]; Christoph H. Borchers[1, 2]; *[1]Dept. of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; [2]University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada*

ThP 631 **Structural Mapping of Atypical Chemokine Receptor 3 by Mass Spectrometry**; Liwen Wang[1]; Martin Gustavsson[2]; Tracy Handel[2]; Irina Kufareva[2]; Mark R. Chance[1]; *[1]Case Western Reserve Univ, Cleveland, OH; [2]University of California San Diego, San Diego, CA*

ThP 632 **The Aggregation Mechanism of a Naturally Occurring Highly Amyloidogenic β2-Microglobulin Variant Probed Using Structural Mass Spectrometry**; Owen Cornwell[1]; Sheena E Radford[1]; Alison E Ashcroft[1]; *[1]University of Leeds, Leeds, Yorkshire*

ThP 633 **Proteolytic MALDI Compatible Chips for Limited Proteolysis and H/D Exchange Analysis**; Michal Rosulek[1, 2]; Petra Darebna[1, 2]; Lukas Slavata[1, 2]; Michael Volny[3]; Petr Man[1, 2]; Petr Pompach[1, 3]; Petr Novak[1, 2]; *[1]BIOCEV, Institute of Microbiology of the CAS, v.v.i., Vestec, Czech Republic; [2]Faculty of Science, Charles University, Prague, Czech Republic; [3]AffiPro s.r.o., Mratin, Czech Republic*

ThP 634 **The C-type Lectin-Like Receptor Nkrp1b: Important Structural Features in the Context of Protein Conformation and Interactions**; Lucie Hernychova[1, 2]; Michal Rosulek[2, 3]; Ljubina Ivanova[2]; Valeria Grobarova[1]; Ondrej Sebesta[1]; Alan Kadek[2, 3]; Josef Chmelik[4]; Kristian Skala[2]; Zdenek Kukacka[2, 3]; Jan Cerny[1]; Petr Novak[2, 3]; *[1]Department of Cell Biology, Faculty of Science, Charles University, Prague, Czech Republic; [2]BIOCEV, Institute of Microbiology of the CAS, v.v.i., Vestec, Czech Republic; [3]Department of Biochemistry, Faculty of Science, Charles University, Prague, Czech Republic; [4]Institute of Microbiology of the CAS, v.v.i., Prague, Czech Republic*

ThP 635 **Utilizing 193 nm UVPD for Identification of Peptide Crosslinks to Characterize Protein Interactions**; Michael Cammarata[1]; Sarah Sipe[1]; Jake Rosenberg[1]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

ThP 636 **Structural Characterization of Protein by Using Enzymatic Reactor**; Grifnée Elodie[1]; Hanozin Emeline[1]; Smargiasso Nicolas[1]; Quinton Loïc[1]; Mazzucchelli Gabriel[1]; De Pauw Edwin[1]; *[1]Mass Spectrometry Laboratory, Liège, Belgium*

ThP 637 **Complex Conformations: Ion Mobility Mass Spectrometry Provides Insight into a Conformationally Dynamic Protein Complex**; Sophie R Harvey[1]; Varun V Gadkari[1]; Zucai Suo[1]; Vicki H Wysocki[1]; *[1]The Ohio State University, Columbus, OH*

ThP 638 **Exploring Two-State Cooperative Protein Folding Using Ion Mobility Spectrometry-Mass Spectrometry**; Shannon A Raab[1]; Tarick J El-Baba[1]; Daniel W Woodall[1]; Wen Liu[2]; Yang Liu[2]; Arthur Laganowsky[2]; David H Russell[2]; David E Clemmer[1]; *[1]Indiana University, Bloomington, IN; [2]Texas A&M University, College Station, Texas*

ThP 639 **Probing Ligand-Induced GPCR Conformational Changes by In-Cell Crosslinking and Mass Spectrometry** ; Bill Huang[1]; Ji-Won Lee[1]; Hee-Yong Kim[1]; *[1]NIAAA/NIH, Rockville, MD*

ThP 640 **Structural Comparisons of Trimeric Phospholipase A2 from Australian Snake Venoms**; Julian A. Harrison[1, 2]; Celine Kelson[1, 2]; Jenny L. Beck[1, 2]; *[1]School of Chemistry, University of Wollongong, Wollongong, Australia; [2]Illawarra Health and Medical Research Institute, University of Wollongong, Wollongong, Australia*

ThP 641 **Investigating the Dynamics and Assembly of alpha-Synuclein Amyloid Oligomers by ESI-IMS-MS**; Rebecca Mason[1]; Caroline Dalton[1]; David Smith[1]; *[1]Biomolecular Sciences Research Centre, Sheffield Hallam University, Sheffield, UK*

ThP 642 **Quantitative Protein Topography Measurements by High Resolution Hydroxyl Radical Protein Footprintingfor Molecular Modeling**; Boer Xie[1]; Amika Sood[1]; Robert J. Woods[1]; Joshua S. Sharp[2]; *[1]Complex Carbohydrate Research Center, University of Georgia, Athens, GA; [2]University of Mississippi, University, MS*

ThP 643 **Integrative MS-based Biophysical Methods Show the Bridging Two Domains is a Mechanism for catalysis of OCP by FRP**; Yue Lu; *Washington University, St. Louis, St Louis*

ThP 644 **Delivering Transmembrane Peptide Complexes to the Gas Phase Using ESI and Nanodiscs**; Jun Li[1]; Michele R. Richards[1]; Elena Kitova[1]; John Klassen[1]; *[1]University of Alberta, Edmonton, AB, Canada*

ThP 645 **Advancing Synchrotron X-Ray Protein Footprinting through Radiolysis Chemistry and Post-Exposure Treatments**; Simin D. Maleknia[1]; Sayan Gupta[2]; Corie Ralston[2]; *[1]University of New South Wales, Sydney , NSW; [2]Lawrence Berkeley National Laboratory, Berkeley, CA*

ThP 646 **Proteome Thermostability in the Bacillaceae Family**; Jeremy Volkening[1]; Pei Liu[1]; Greg Sabat[1]; Michael R. Sussman[1]; *[1]University of Wisconsin-Madison, Madison, WI*

ThP 647 **Epitope and Paratope Mapping of Virus-Antibody Complexes**; Ganesh S. Anand[1]; Xin Xiang Lim[2]; Arun Chandramohan[2]; *[1]NUS Singapore, Singapore; [2]National University of Singapore, Singapore, Singapore*

ThP 648 **A Traveling Wave Ion Mobility Spectrometry and Molecular Modeling Study of Heparin/HS-Protein Interactions for Robo1**; Yuejie Zhao[1]; Jeong Yeh Yang[2]; Yongmei Xu[3]; David Thieker[2]; Chengli Zong[2]; Kelley Moremen[2]; Jian Liu[3]; Geert-Jan Boons[2]; Robert Woods[2]; I.Jonathan Amster[1]; *[1]University of Georgia,Chemistry Department, Athens, GA; [2]Complex Carbohydrate Research Center, University of Georgia, Athens, GA; [3]University of North Carolina, Chapel Hill, NC*

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ThP 649 **High Resolution Protein Profiling of Aortic Valves with and without Left-Ventricular Assist Device (LVAD) Implantation**; Hemanth Akkiraju[1]; Lewis M. Brown[1]; Elizabeth H. Stephens[1]; Jiho Han[1]; Emma Trawick[1]; Gordana Vunjak-Novakovic[1]; Hiroo Takayama[1]; *[1]Columbia University, New York , NY*

ThP 650 **Identification of Rare Hemoglobin Variant by Mass Spectrometry**; Shawn Connolly[1]; Thomas Everett[1]; Steven Hanson[1]; Kuanysh Kabytaev[1]; *[1]University of Missouri, Columbia, MO*

ThP 651 **Phospho-Barcodes of Renal Cell Carcinoma Cell Lines Reveals Differential Mechanisms in Sunitinib Resistance**; Shao-Kuan Chen[1, 2]; Chi-Jung Huang[2, 3]; Yen-Chieh Wang[1, 2]; Tai-Yuan Lin[1]; Wei-Chi Ku[1]; *[1]fu Jen Catholic University, New Taipei City, Taiwan; [2]Cathay General Hospital, Taipei, Taiwan; [3]National Defense Medical Center, Taipei, Taiwan*

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