

# Journal of the American Society for Mass Spectrometry

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# 69<sup>th</sup> Conference on Mass Spectrometry and Allied Topics



**October 31 - November 4, 2021** Philadelphia, Pennsylvania



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Welcome to the 69th ASMS Conference on Mass Spectrometry and Allied Topics. Conference program activities and exhibit booths are in the Pennsylvania Convention Center.



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**Teledyne Signal Processing Devices** 

# **PROGRAM HIGHLIGHTS**



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

## SUNDAY SPECIAL KEYNOTE LECTURE 5:00 - 5:45 PM Ballroom B



Race and Gender Discrimination in STEM: Intersecting Oppressions with Multifaceted Solutions

Asia Eaton Florida International University

# SUNDAY TUTORIAL SESSIONS 5:45 - 6:45 PM Tutorial Session I, 5:45-6:45 PM, Ballroom B



Applications of Mass Spectrometry for Clinical Diagnostics: The Influence of Turnaround Time

Abraham Badu-Tawiah The Ohio State University

# Tutorial Session II, 5:45-6:45 PM, Ballroom A



Annotation of Mass Spectrometry Metabolomics Data

Jessica Prenni Colorado State University

# SUNDAY CONFERENCE OPENING 6:45 - 7:45 PM Ballroom B



WELCOME

Julia Laskin Purdue University ASMS Vice President for Programs



Epigenetic Pathways as Targets in Human Health and Disease

Shelley L. Berger University of Pennsylvania

SUNDAY WELCOME RECEPTION 7:45 - 9:00 PM Poster-Exhibit Hall Sponsored by Thermo Fisher Scientific

### Monday Award Lecture 4:45 - 5:30 PM Ballroom B



Fenn Award for a Distinguished Contribution in Mass Spectrometry

Peter B. Armentrout University of Utah

TUESDAY AWARD LECTURE 4:45 - 5:30 PM Ballroom B



Biemann Medal

Nuno Bandeira University of California, San Diego

Wednesday ASMS Meeting 4:45 - 5:30 PM Ballroom B

Enjoy a beverage, hear ASMS Board reports and applaud award recipients.

#### THURSDAY PLENARY SESSION 4:45 - 5:30 PM Ballroom B



Computer Vision and the Neural Network Revolution

William T. Freeman Massachusetts Institute of Technology

**THURSDAY FAREWELL TOAST & RECEPTION 5:30 - 7:30 PM** Grand Hall Sponsored by Shimadzu Scientific Instruments



Consult online planner or mobile app for detailed program. Also includes content for in-person and remote posters.



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

All oral sessions will be broadcast live and recording available for the benefit of both in-person and remote attendees.

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

**IN-PERSON SPEAKERS** must load presentations at least one day prior to their talks. The speaker ready room is 203 AB. 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

**IN-PERSON POSTERS AND EXHIBIT BOOTHS**, Hall A-B. The Hall is open:

Sunday Welcome Reception ....7:45 pm - 9:00 pm Monday - Wednesday ......7:00 am - 8:00 pm Thursday .......7:00 am - 2:30 pm

**IN-PERSON 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.

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

**IN-PERSON POSTER AUTHORS** must be present at posters on scheduled days at these times. This schedule allows for a one-hour non-overlapping lunch break. All presenters are now scheduled for 3 hours (authors are welcome to attend the full four hours).

**Odd-number posters present:** 10:30 am - 11:30 am PLUS 12:30 – 2:30 pm

**Even-number posters present:** 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm

#### Poster Pick-Me-Up Snacks served at 1:30 pm.

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. **REMOTE POSTERS** are available for viewing in the online planner and mobile app.

**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. Follow signs from the Grand Hall to Reading Terminal Market for more tasty lunch options.

**WORKSHOPS** are 5:45 - 7:00 pm on Monday, Tuesday, and Wednesday. Workshop presenters should bring their presentations to the workshop session room. USB stick with presentation is preferred. Light refreshments are provided.

**FREE WIFI Access** is 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.

**Recordings** includes tutorial lectures, plenary lectures, and oral sessions. Recordings will be available to conference attendees for three months after the conference via the mobile app and online planner. ASMS does not retain rights to material included in web casts.

**CAREER CENTER** will be online only this year. Please visit ASMS.org to access the Career Center.

GENDER NEUTRAL RESTROOMS are available.

**MAMAVA/LACTATION PODS** Two pods are located in the convention center (in concourse between Halls A and B and also in Broad St Atrium.) Download the free Mamava app from app stores to unlock these lactation suites.

#### **CONFERENCE HOTELS**

Philadelphia Marriott, 1201 Market Street, Phila, PA 19107 Tel: 215-625-2900

The Notary Hotel, 21 N. Juniper, Phila, PA 19107 Tel 215-496-3200

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Consult online planner or mobile app for detailed program. Also includes content for in-person and remote posters.



# **CODE OF CONDUCT**

The ASMS Code of Conduct guides the expected, professional behavior of all participants at conferences, short courses, and conference-related activities and events, regardless of whether your registration is submitted by you or your proxy.

#### ACCEPTABLE BEHAVIOR INCLUDES:

- · Treating everyone with respect and consideration;
- Communicating openly and thoughtfully with others and being considerate of the multitude of views and opinions that may be different from your own;
- Being respectful and mindful in your critique of ideas;
- · Being mindful of your surroundings and of your fellow participants.

#### **UNACCEPTABLE BEHAVIOR INCLUDES:**

- Harassment and intimidation, including any verbal, written, or physical conduct designed to threaten, intimidate, or coerce any
  participant, speaker, exhibitor, conference or event organizer or staff, service provider, volunteer, or guest;
- Discrimination based on gender or gender identity, sexual orientation, age, disability, physical appearance, body size, race, religion, national origin, culture, or any other characteristic provided by law;
- Physical or verbal abuse of any participant, speaker, exhibitor, conference or event organizer or staff, service provider, volunteer, or guest;
- Threats of physical violence against any participant, speaker, exhibitor, conference or event organizer or staff, service provider, volunteer, or guest; and
- Disrespectful disruption of presentations.

#### **CONSEQUENCES OF UNACCEPTABLE BEHAVIOR:**

Anyone who violates this Code may be subject to the below consequences. ASMS reserves the right to take action beyond these consequences as necessary based on a participant's behavior in violation of the Code.

- · Anyone requested to stop unacceptable behavior is expected to comply immediately;
- · Immediate removal from the meeting or event without warning and potentially without refund; and/or
- Prohibition from attending future meetings or events in the sole determination of ASMS.

#### **WHO TO CONTACT:**

ASMS Executive Director, Jennifer Watson, jennifer@asms.org

ASMS is proud of our annual conferences, short courses, and conference-related events and wants everyone to have a positive learning and networking experience. Embracing the above professional behavior will help ensure a great experience for all involved.

Text adapted from https://www.frontiersin.org/articles/10.3389/fmars.2016.00103/full Favaro Brett, Oester Samantha, Cigliano John A., Cornick Leslie A., Hind Edward J., Parsons E. C. M., Woodbury Tracey J., "Your Science Conference Should Have a Code of Conduct", Frontiers in Marine Science, 2016, 3, 103

# **CONFERENCE REGULATIONS**

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

- Name badge, verification of vaccination, and negative covid test are required to enter the conference..
- No smoking is permitted in the convention center.
- All devices must be silent and screens darkened in oral sessions.
- No photography or recording is allowed in oral sessions or in the poster/exhibit Hall.
- **Material presented or displayed** at the ASMS Conference, including but not limited to talks, 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 exhibitor events.
- No organized activities (even off-site) other than those approved by ASMS are allowed during the conference week (5:00 pm on Sunday through 6:00 pm on Thursday).
- Corporate or institutional logos on slides or posters may appear only one time in the presentation.
- Parents. Due to the health & safety plan in place for the conference we do not suggest bringing children.



# **BLOCKBUSTER YEAR FOR NEW HISTORY POSTERS**

The ASMS History Committee looks forward to providing 2021 annual conference attendees with yet another fascinating array of insights into the evolution of the practice of mass spectrometry and the history of the Society. The history poster display, located in the 'Bridge' connecting the Grand Hall Registration area and the Poster-Exhibit Hall, promises to be a convenient and welcoming venue for learning and discussion. Fueled by ASMS members' shared but often disparate memories, conversations around the history posters are always lively. Do plan to spend some time with us!



Sir J. J. Thomson

The use of mass spectrometers as analytical instruments was envisioned by J. J. Thomson in his 1913 monograph "Rays of Positive Electricity and their Application to Chemical Analysis." And yet it wasn't until the 1940s that commercial production of the new instruments began. First to market were CEC, GE, and Westinghouse in the US, Metropolitan Vickers in the UK, and MAT in Germany. By the 1950s, they were joined by JEOL and Hitachi in Japan. Using posters prepared primarily by current vendors, our **Vendor History display** continues the story. The History Committee is delighted this year to showcase 2020 contributions from Kratos, Shimadzu, Waters TOF.

With the **History of Applications** display, we begin an exploration of the enormous variety of ways in which mass spectrometers have been used. The first poster in this series, prepared for the 2020 conference, describes ways in which mass spectrometry has aided forensic science. Continuing the series in 2021, we will add two more posters: one on the history of environmental applications and the other on the history of the use of mass spec in space exploration. Despite the distinctly different nature

of these fields, mass spectrometry has played - and continues to play - a dominant role in each. Enjoy the richness of these accounts and stay tuned in future years as we explore other fields.

By 2019 the ASMS membership was divided ~60:40 males to females and approximately equally between Caucasian members and members from other racial and ethnic groups. But, as the **History of ASMS Diversity** posters will show, that was not always the case. Early photographs of mass spectrometrists are dominated by male faces, mostly Caucasian, while lists of early publications in the field consist largely of male author names. The Society's transformation began in the 1970s and gained momentum through succeeding decades. Occupations of Society members have also changed: we've gone from a membership dominated by academics and denizens of government labs to one in which most of our members are employed in industry. Carve out some time to spend with these two new posters prepared in collaboration with the Diversity Committee. We think you'll find them chock-full of interesting data and charts!



# NOTABLE PEOPLE IN MASS SPECTROMETRY



Want to learn more about people who have made significant contributions to mass spectrometry? Use the JASMS Obituaries links (www.asms.org/publications/journal-of-theamerican-society-for-mass-spectrometry-group/obituaries-from-jasms) to read tributes to departed colleagues, including a remembrance soon to be published of Ron Grigsby, a founding member of ASMS who worked in the petroleum industry. Videos of Ron in conversation with Mike Grayson and running the CEC instrument he installed in his basement can be found under History Videos on the History web page (www.asms.org/about/history/about-asms-and-ms-history). Want to learn still more? View profiles of three pioneers in the field among the posters on the History web page (www.asms.org/about/history-posters) and follow the link posted there to oral histories archived at the Science History Institute



# **ASMS BOARD OF DIRECTORS**



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Member at Large for Publications Stephen Valentine West Virginia University Morgantown, PA



Member at Large for Digital Communications Francisco Fernandez-Lima Florida International University Miami, FL

#### THANK YOU

to these members who are retiring from the ASMS Board but are continuing to serve for this postponed conference.

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Leslie M. Hicks University of North Carolina Chapel Hill, NC



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Environmental Applications	Paul Chiarelli Andrew Ottens
Exposomics	Silvia Balbo Benedikt Warth
Flavor, Fragrance and Foodstuff	Joe Binkley Travis Falconer
Forensics & Homeland Security	Brittany Casey Ruth Waddell Smith
FTMS	Lissa Anderson Chad Weisbrod
Fundamentals	Alexander Makarov Alexandre Shvartsburg
H/D Exchange, Covalent Labeling & Cross Linking	Fabio Gozzo Miklos Guttman
Imaging MS	Angus Grey Tiffany Porta
Ion Mobility MS	Kelly Hines Ian Webb
lon Trap MS	Theresa Evans-Nguyen Dalton Snyder
LC/MS Related Topics	Kendra Adams Erik Soderblom
Lipids & Lipodomics	Michael Holčapek Harald Köfeler
Metabolomics	Maryam Goudarzi Thomas Horvath
Native MS	lain Campuzano Michael Marty
Pharmaceuticals	Angela Calderon Glenn Harris
Photoionization MS	Luke Hanley Matthias Lorenz
Polymeric Materials	Thierry Fouquet Jessica Hoskins

Regulated Bioanalysi	is	Dian Su Jian Wang
Top-Down Proteomic	S	Joe Cannon Caroline DeHart
Undergradua Research in N	nte 1S	Matt Joyner Kate Stumpo
Young Ma Spectrometris	ss sts	Christopher Rose Laura Sanchez
Co	OMN	IITTEES
Asilomar Conference (ACMS)	Jas Joł Be Ric	son Hogan, Chair nn Bowden atrix Ueberheide chard Yost (ASMS Board Rep.)
Audit	Pa Ke Yin Ljilj	trick Griffin, Chair vin Bateman ıg Ge jana Pasa-Tolic
Corporate Liaison	Mic Jer Na Ma Ang Lau	chael Easterling (ASMS Board Rep.) chael Barrett Anderson, Evosep nnifer Copeland, VICI Para, Newomics nureen Quaranta, Shimadzu gie Jinks, Thermo Fisher Scientific uryn Bailey, SCIEX
Digital Communications	Fra Birg De The Xin	ancisco Fernandez-Lima, Chair git Schilling vin Schweppe omas Wales y Yan
Diversity & Inclusion	Ca Jer Sa Do Ca Ric	ndice Ulmer, Chair nnifer Campbell iful Chowdhury minic Gostick rlos Larriba Andaluz chard Yost (ASMS Board Rep.)
Education	Lis Alli Bol Jos Lis	a Jones, Chair son Scott bby Basu seph Eschweiler a O'Callaghan
History	P. Asl Ro Ma Adi Mic	Jane Gale, Chair her Newsome n Hites ignus Palmblad rienne Tymiak chael Grayson, <i>ex-officio</i>
Nominating	Jer Tar Lar Ch Tot	nnifer Brodbelt, Chair run Anumol n Huang ristina Jones uradji Solouki
Publications	Ste Ric Var Si V Mo Jos	ephen Valentine, Chair chard Y. Huang nessa Phelan Wu wei Zhou seph Loo, <i>ex officio</i>
Sanibel Conference	Lis Xiu Ric Ljilj	sa Anderson, Chair ixia Du chard Rogers jana Pasa-Tolic (ASMS Bd Rep.)



#### JOHN B. FENN AWARD FOR A DISTINGUISHED CONTRIBUTION IN MASS SPECTROMETRY 2021 Recipient: Peter B. Armentrout Award Lecture: 4:45 PM, Monday, Ballroom B



The ASMS Award for Distinguished Contribution in Mass Spectrometry honors the memory of John B. Fenn who shared the 2002 Nobel Prize for the development of electrospray ionization. John joined ASMS in 1986 and remained an active member until his passing in 2010. The award is conferred at the ASMS Annual Conference with the presentation of a \$10,000 cash award, a recognition plaque, and the award lecture.

**Dr. Peter B. Armentrout** is the 2021 recipient of the ASMS John B. Fenn Award for a Distinguished Contribution in Mass Spectrometry, for the development of robust experimental and statistical techniques for the determination of accurate thermochemistry. He developed the guided ion beam threshold dissociation approach to provide insights into the thermochemistry, kinetics, and dynamics of simple and complex chemical

reactions. In addition, he developed a suite of software programs for statistically modeling the energy dependence of product formation for most reactive processes. He shared both the instrumentation designs and the software with labs around the world to enable the greater scientific community to study thermochemical processes.

These developments have allowed nearly 2500 distinct bond energies to be measured during his career. The impact of these fundamental measurements has been felt over many fields, including catalysis, biochemistry, surface chemistry, organometallic chemistry, and plasma chemistry.

Dr. Armentrout is the Henry Eyring Presidential Endowed Chair of Chemistry, University of Utah.

# AL YERGEY MS SCIENTIST AWARD 2021 Recipients Award Presentations: 4:45 PM, Monday, Ballroom B



The AI Yergey Mass Spectrometry Scientist Award is sponsored by ASMS to recognize dedication and significant contributions to mass spectrometry-based science by "unsung heroes. This award is named in memory of AI Yergey a well-respected scientist who was known as a dedicated mentor.

**Dr. Mark Kushnir** is one of two recipients of the 2021 Al Yergey MS Scientist Awards. He is the Scientific Director for Mass Spectrometry Research and Development at the ARUP Institute for Clinical and Experimental Pathology. He spearheaded the adoption of tandem mass spectrometry by ARUP Laboratories and has done exemplary work on developing mass-spectrometry-based clinical assays to be used for patient care, including using desalting columns to purify unbound molecules from plasma samples, leading to a clinical assay for

25-hydroxyvitamin D. He has published more than 100 papers and also been involved with discovery projects and scientific collaborations with many researchers.

Dr. Kushnir has mentored countless people, including R&D colleagues, clinical chemistry fellows and pathology residents. He is an editorial Board Member for many publications and is a regular reviewer for clinical chemistry and analytical chemistry journals and organizations.



**Dr. Arpad Somogyi** is recipient of the second 2021 AI Yergey MS Scientist Award. He is Associate Director of MS&P facility at the Ohio State University. He has been involved in key research areas including instrument design related to SID, small molecule analysis by FT-ICR, the study of fragmentation mechanisms of protonated peptides, and the structural investigation of proteins and protein substrate interactions. He has authored over 125 scientific publications.

Dr. Somogyi has mentored countless graduate students and post-doctoral fellows. He served as an instructor at an ASMS 2-day short course for 10 years. He also contributes to multiple OSU credit courses and regularly reviews for journals in areas of fundamental topics.

## **ASMS AWARDS**



#### BIEMANN MEDAL 2021 Recipient: Nuno Bandeira Award Lecture: 4:45 PM, Tuesday, Ballroom B



The Biemann Medal is awarded to an individual early in his or her career to recognize significant achievement in basic or applied mass spectrometry. The Medal is conferred at the ASMS Annual Conference with the presentation of a \$5,000 cash award, a recognition plaque, and the award lecture.

**Dr. Nuno Bandeira** is the 2021 recipient of the ASMS Biemann Medal for significant contributions regarding the development of spectral alignment to connect the world's mass spectrometry data that is leading to the development of a data driven Google-type search engine for mass spectrometry data. Dr. Bandeira realized that similar to the alignment of protein sequences, unidentified MS/MS spectra can be aligned for the identification of modified and unmodified variants of the same peptide. It can also be applied to small

molecules to identify drug-related metabolites or analogs.

In order to improve the efficiency of searching these data repositories, Dr. Bandeira created the foundation of a Google search network by precomputing the large-scale network of all available MS/MS data in the MassIVE public mass spectrometry data repository. The master spectral network can now be searched using data instead of text. These molecular networks have been used in hundreds of papers and have been key to understanding mechanisms of metabolic exchange and charting the molecular diversity in human food and habitats, across kingdoms and many microbial species.

Dr. Bandeira is Associate Professor of Computer Science and Engineering at the Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California at San Diego.

# 2021 RESEARCH AWARDS Award Presentations: 4:45 PM, Tuesday, Ballroom B

Research awards promote the research of academic scientists within the first four years of joining the tenure track or research faculty of a North American University at the time the award is conferred. The awards, in the amount of \$35,000 each, are fully supported by Bruker, Thermo Fisher Scientific, and Waters Corporation.

Sponsored by BRUKER



Yansheng Liu Yale University

Sponsored by THERMO FISHER SCIENTIFIC



Luca Fornelli University of Oklahoma

Sponsored by WATERS CORPORATION



Xin Yan Texas A&M University

#### 2021 PRIMARILY UNDERGRADUATE INSTITUTION RESEARCH AWARD Award Presentations: 4:45 PM, Tuesday, Ballroom B



#### **S**PONSORED BY **A**GILENT **T**ECHNOLOGIES

This award promotes academic research in mass spectrometry by faculty members and their students at primarily undergraduate institutions (PUIs). The award of \$20,000 is made to the recipient's institution on behalf of the recipient's research.

Christopher Mulligan Illinois State University





## RON HITES AWARD OUTSTANDING RESEARCH PUBLICATION IN JASMS Award Presentations: ASMS Meeting, 4:45 PM, Wednesday, Ballroom B



The Ron Hites Award is for 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 2021 Ron Hites Award recognizes **Michael T. Marty**, University of Arizona, and co-authors Marius M. Kostelic, Alex M. Ryan, Deseree J. Reid, and Jibriel M. Noun for their paper "Expanding the Types of Lipids Amenable to Native Mass Spectrometry of Lipoprotein Complexes" (*J. Am. Soc. Mass Spectrom.* (2019) **30**:1416Y1425).

# 2021 POSTDOCTORAL CAREER DEVELOPMENT AWARDS Award Presentations: ASMS Meeting, 4:45 PM, Wednesday, Ballroom B

Up to five awards in the amount of \$5,000 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.



Hilary Brown Naval Air Warfare Center



Mahmud Iqbal University of Florida



**Sylwia Stopka** The Brigham Young Women's Hospital



Fernando Tobias The Ohio State University



Matthew Waas Princess Margaret Cancer Centre





# 2021 STUDENT TRAVEL AWARDS

Award Presentations: ASMS MEETING, 4:45 PM, WEDNESDAY, BALLROOM B

#### 2021 GRADUATE STUDENT TRAVEL AWARDS

Linda Berg Luecke, Medical College of Wisconsin Valentine Courouble, Scripps Research Institute Roshan Javanshad, Western Michigan University Benjamin Jones, The Ohio State University Carter Lantz, University of California Los Angeles Yangjie Li, Purdue University Yiran Liang, Brigham Young University Laura Muehlbauer, University of Wisconsin-Madison Thao Nguyen, Princeton University Melanie Odenkirk, North Carolina State University Crystal Pace, North Carolina State University Deanna Plubell, University of Washington Deseree Reid, University of Arizona David Roberts, University of Wisconsin-Madison Patric Sadecki, UNC - Chapel Hill Ian Smith, University of Washington Dylan Tabang, University of Wisconsin Shuli Tang, Texas A&M University Daisy Unsihuay, Purdue University Tim Van Den Bossche, Ghent University

#### 2021 UNDERGRADUATE STUDENT TRAVEL AWARDS

Nancy Abdelrahman, North Carolina State University Ashish Chakraborty, University of Texas at Austin Wenya Jian, Univ. of North Carolina at Chapel Hill Tsach Mackey, Georgetown University Rajendra Panth, Western Michigan University Alicia Plourde, University of Guelph Qiuwen Quan, University of Wisconsin-Madison Caroline Roycroft, University of Wisconsin-Madison Anna Rullan Buxo, Yale University Leighann Weber, James Madison University

## 2020 STUDENT TRAVEL AWARDS Award Presentations: ASMS Meeting, 4:45 pm, Wednesday, Ballroom B

The 2020 student travel awards were not distributed for the virtual conference. These students still meet the eligibility requirements will receive the travel funds to attend this 2021 conference.

#### 2020 GRADUATE STUDENT AWARDS

Kyle Brown, University of Wisconsin-Madison Edwin Escobar, University of Texas-Austin Elaura Gustafson, Brigham Young University Christian Leritano, Waterloo University Miyang Li, University of Wisconsin-Madison Bailey Rose, Vanderbilt University Pei Su, Purdue University Conner Harper, University of California, Berkeley Allyson Mellinger, North Carolina State University Melissa Pergande, University of Illinois - Chicago Baiyi Quan, Duke University Joshua Salem, University of Michigan Yekaterina Kori, University of Pennsylvania

#### **2020 UNDERGRADUATE STUDENT AWARDS**

Kristie Baker, Florida Institute of Technology Rebecca Cain, Indiana-Purdue Indianapolis



Consult online planner or mobile app for detailed program. Also includes content for in-person and remote posters.





69TH ASMS CONFERENCE ON MASS SPECTROMETRY









# **POSTER / EXHIBIT HALL**





# MEDIA EVENTS (PRESS CONFERENCES)

All members of the press are invited to attend these events.

MONDAY, NOVEMBER 1				
(0	Pennsylvania Conventio	n Center		
DIA	9:30 - 10:30 am	Shimadzu Scientific Instruments	Room 107	
ME	11:00 am - 12:00 pm	SCIEX	Room 105 AB	
	1:30 - 2:30 pm	Agilent	Room 107	

# **BREAKFAST AND DINNER SEMINARS**

Breakfast and Dinner Seminars are hosted by Corporate Members at the Pennsylvania Convention Center.

Pre-registration (RSVP) is recommended because room set-up and catering are arranged in advance. Please look for Breakfast and Dinners Seminars page on www.asms.org and in the online planner / mobile app to find online registration links for these events.

		MONDAY, I	NOVEN	IBER 1
S	Pennsylvania Conventio All breakfasts begin at 7:0	Pennsylvania Convention Center All breakfasts begin at 7:00 AM		
ST	Agilent	Room 120 AB	NNERS	MassTech
AKFA	Biognosys	Room 121 AB		SCIEX
	LECO Corporation	Room 117		Shimadzu
Ш Ш	SCIEX	Room 119 AB	Ō	Thermo F
Ξ	Shimadzu	Room 120 C		
	Thermo Fisher Scientific	Room 118 AB		

II.					
	Pennsylvania Convention Center All dinners begin at 7:00 PM				
	MassTech	Room 117			
	SCIEX	Room 119 AB			
	Shimadzu	Room 120 C			
	Thermo Fisher Scientific	Room 118 C			

TUESDAY, NOVEMBER 2					
S	Pennsylvania Conventio All breakfasts begin at 7:0	n Center 0 AM		Pennsylvania Convention All dinners begin at 7:00 PM	Center ⁄/
L S	Agilent	Room 120 AB	S	908 Devices	Room 117
KFA	PerkinElmer	Room 122 AB	INNER	SCIEX	Room 119 AB
	Pharma Fluidics	Room 121 AB		Shimadzu	Room 120 C
N N	Sapient	Room 115 AB		Thermo Fisher Scientific	Room 118 C
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Ξ	Shimadzu	Room 120 C			
	Thermo Fisher Scientific	Room 118 AB			

WEDNESDAY, NOVEMBER 3					
Pennsylvania Convention Center All breakfasts begin at 7:00 AM		S	Pennsylvania Convention Center All dinners begin at 7:00 PM		
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	Biognosys	Room 121 AB		SCIEX	Room 119 AB
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	Thermo Fisher Scientific	Room 118 AB			

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BRE	Thermo Fisher Scientific	Room 118 AB		remot

Consult online planner or mobile app for detailed program. Also includes content for in-person and remote posters.

# ASMS CORPORATE MEMBERS

Corporate Member	Exhibit Booth	Other
908 Devices	306	Meal Seminar(s), see pg 16
ACS/Labs	827	Corporate Poster
Adaptas Solutions	807	
Advanced Materials Technology	606	
Advion	918	
Affinisep USA	321	Corporate Poster
AffiPro		
Agilent Technologies	701	Corporate Poster; Meal Seminar(s), see pg 16
AIM Research Company	124	
Alliance Pharma	603	
Analytical Sales and Services, Inc.		
ANCORP	107	Corporate Poster
Anest Iwata Air Engineering	524	
Antec Scientific		
Aspect Analytics	813	
BaySpec, Inc.	309	
BGI Americas	214	Corporate Poster
Biocrates Life Sciences AG	724	
Biognosys	224	Meal Seminar(s), see pg 16
Bioinformatics Solutions Inc.	315	Corporate Poster
Biotage	324	
Biotech Support Group	206	
Bruker Daltonics	719	Corporate Poster

Corporate Member	Exhibit Booth	Other
Cambridge Isotope Laboratories, Inc.		
Cayman Chemical Company	225	Corporate Poster
CDS Analytical, LLC	115	
Cellenion	725	Corporate Poster; Meal Seminar(s), see pg 16
Cerno Bioscience	614	
CoAnn Technologies		
CovalX	515	
Covaris	607	Corporate Poster
Edwards Vacuum	509	
El-Mul Technologies	512	
e-MSion, Inc.	413	
ESI Source Solutions	207	
Evosep	313	Corporate Poster
Excellims Corporation	125	
F-DGSi	806	
Finneran Porvair	702	
Gene Era Biosciences, Co., Ltd.	926	
Genedata	407	
GenNext Technologies, Inc.	424	
Genovis Inc	119	
GlycoPath	325	
Hamilton Company	113	Corporate Poster
HTX Technologies, LLC	815	Corporate Poster
IMCS	513	

<u>Philadelphia</u>

# **ASMS CORPORATE MEMBERS**

Corporate Member	Exhibit Booth	Other
INFICON	602	
International Equipment Trading Ltd	108	
InterVenn Biosciences	202	
Ion Opticks Pty Ltd	819	
IonBench	312	
IonDX		
lonoptika Ltd.		
lonsense Inc.	601	Corporate Poster
IROA Technologies LLC	700	
JEOL USA, Inc.	801	Corporate Poster
Larodan	120	
LECO Corporation	600	Corporate Poster
Leybold USA	100	
Linden CMS GmbH	418	
LNI Swissgas	915	
Mass Analytica	409	
Masspeclink Technologies, LLC	627	
MassTech Inc.	121	Corporate Poster; Meal Seminar(s), see pg 16
Matrix Science	327	
McKinley Scientific		
Mestrelab Research	612	
MetaSci Inc.	307	
MOBILion Systems, Inc.	707	Corporate Poster; Meal Seminar(s), see pg 16
MPF Products Inc	109	
MRM Proteomics	706	

Corporate Member	Exhibit Booth	Other
msAld GmbH	301	Corporate Poster
MSTM, LLC	227	
National Institute of Standards and Technology (NIST)	319	
Nest Group, Inc., The		
Newomics Inc.	821	
NXT Power	212	
Omics Informatics	508	Corporate Poster
Omni International	106	
Optimize Technologies	200	Corporate Poster
Parker Hannifin	615	
Peak Scientific	519	Corporate Poster
PerkinElmer, Inc.	412	Meal Seminar(s), see pg 16
Pfeiffer Vacuum	415	Corporate Poster
PharmaFluidics	213	Corporate Poster; Meal Seminar(s), see pg 16
Phenomenex	526	
Phoenix S&T, Inc.	506	
Photonis	619	Corporate Poster
Phytronix Technologies	400	
Plasmion	713	Corporate Poster
PreOmics GmbH	715	Corporate Poster
Prolab Instruments GmbH	708	Corporate Poster
Protein Metrics Inc.	514	
Proteoform Scientific	303	
Proteome Software Inc.	507	

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Corporate Member	Exhibit Booth	Other
ProtiFi, LLC	825	
Rapid Novor Inc.	118	
Refeyn Inc.	427	
Regis Technologies	208	
Restek Corporation	218	
ReSyn Biosciences	726	
Sapient	903	Meal Seminar(s), see pg 16
Schivo Medical	808	
SCIEX	401	Meal Seminar(s), see pg 16
Seer	824	
SepSolve Analytical Ltd.	914	
Shimadzu Scientific Instruments, Inc.	419	Meal Seminar(s), see pg 16
Shimifrez Inc.	625	
Shodex - Showa Denko America	907	
Sierra Analytics	525	Corporate Poster
Silantes	225	
Sound Analytics		
South Tek Systems	912	

Corporate Member	Exhibit Booth	Other
Southeast Center for Integrated Metabolomics	626	Corporate Poster
Spark Holland B. V.		
Spectroswiss	501	
Spellman High Voltage Electronics Corp.	613	
Tecan	924	
Teledyne Signal Processing Devices		
The Metabolomics Innovation Centre	712	
Thermo Fisher Scientific	201	Meal Seminar(s), see pg 16
Tosoh Bioscience LLC	426	
Trace Matters	112	
Trajan Scientific and Medical	102	
Verdel Instruments	714	
VICI	406	Corporate Poster
vivitide	127	
Waters Corporation	219	
XP Power LLC	101	
Xtreme Power	901	
Zef Scientific, Inc.	402	

ASMS is grateful for the support of all Corporate Members. Technologies and services developed by these companies are vital to the ASMS community and the field of mass spectrometry.

Thank you!



#### VICE PRESIDENT FOR PROGRAMS



#### Julia Laskin Purdue University Vice President for Programs

#### **STUDENT ASSISTANTS**

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

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Yina Liu

Pei Su Weiguo Andy Tao Fernando (Ralph) Tobias Daisy Unsihuay Thomas Wales Nicolas Young Haihong Zhou

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Christopher G. Gill Timothy Griffin Alyssa Hansen Ling Hao Kelly Hines W. Scott Hopkins Lisa Jenkins Lisa Jones Kaveh Jorabchi Ryan Julian Desmond Kaplan **Christine Kirkpatrick** Ruwan Kurulugama Ingela Lanekoff Franklin Leach III Anyin Li

Phillip Mach Nicholas Manicke Katy Margulis Jody C. May Rafael Montenegro-Burke Olga Ovchinnikova Malvina Papanastasiou Amanda Patrick Elizabeth Pierson JC Poutsma Dil Ramanathan James Redwine Elena Romanova Christopher Rose David Schroeder

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# **PROGRAM OVERVIEW**



# SATURDAY

9:00 ам - 4:30 рм	Short Courses	
2:00 - 5:00 PM	REGISTRATION, Grand Hall	

# SUNDAY

9:00 ам - 4:30 рм	SHORT COURSES		
10:00 ам - 8:00 рм	REGISTRATION, Grand Hall		
5:00 - 5:45 рм	KEYNOTE LECTURE, Ballroom B		
	Race and Gender Discrimination in STEM: Intersecting Oppressions with Multifaceted Solutions         Asia Eaton         Florida International University		
5:45 - 6:45 рм	TUTORIAL SESSIONS Tutorial Session I, 5:45-6:45 PM, <i>Ballroom B</i>		
	Applications of Mass Spectrometry for Clinical Diagnostics: The Influence of Turnaround Time Abraham Badu-Tawiah The Ohio State University Tutorial Session II. 5:45-6:45 PM. Ballroom A		
	Annotation of Mass Spectrometry Metabolomics Data Jessica Prenni Colorado State University		
6:45 - 7:45 рм	Conference Opening, Ballroom B		
	Julia Laskin, University of South Carolina ASMS Vice President for Programs		
	<b>7:00 - 7:45 PM</b> Epigenetic Pathways as Targets in Human Health and Disease <b>Shelley L. Berger</b> University of Pennsylvania		
7:45 - 9:00 рм	WELCOME RECEPTION, Poster-Exhibit Hall Sponsored by Thermo Fisher Scientific		



### 7:00 AM CORPORATE BREAKFAST SEMINARS, Convention Center (see page 16 for details) 7:30 ам - 5:00 рм **REGISTRATION, Grand Hall** 8:30 - 10:30 AM **ORAL SESSIONS** MOA am Instrumentation: Ambient Ionization and Applications; Ballroom A MOB am Top Down Protein Analysis; Ballroom B MOC am Clinical Analysis: Innovations; 201 ABC MOD am Informatics: Data-Independent Acquisition; 204 ABC MOE am Glycomics; 103 ABC MOF am Fundamentals Beyond Mass Analysis: Structural Characterization of Isomers; 108 AB MOG am Industry: Sample Preparation, Automation, and Quality Control; 113 ABC MOH am Food Safety & Chemistry: Innovations; Room 114 10:30 AM - 2:30 PM POSTER SESSION AND EXHIBITS, Monday Posters, Hall AB Odd-number posters present: 10:30 am - 11:30 am PLUS 12:30 - 2:30 pm Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm 11:30 am - 1:00 pm: Undergraduate students look for reserved tables and free lunch vouchers to Meet the Experts 2:30 - 4:30 рм **ORAL SESSIONS** MOA pm Instrumentation: Portable and Transportable Mass Spectrometers; Ballroom A MOB pm Biotherapeutics: Characterization and Quantitation; Ballroom B MOC pm Metabolomics: Untargeted Profiling; 201 ABC MOD pm Ion Mobility: New Developments & Applications; 204 ABC MOE pm Cancer Research; 103 ABC MOF pm Fundamentals: Unconventional Approaches in MS; 108 AB MOG pm Environmental: Innovative Approaches and Instrumentation; 113 ABC MOH pm GC/MS: Instrumentation and Applications; Room 114 4:45 - 5:30 РМ Award Lecture, Ballroom B Award for a Distinguished Contribution in Mass Spectrometry Peter B. Armentrout University of Utah 5:45 - 7:00 рм **WORKSHOPS** There are light refreshments in foyers, 5:30 - 5:45 pm. 01 Kahoot! Interactive Trivia on LC-MS Related Topics, Ballroom A 02 Machine Learning: How Is It Enhancing Mass Spectrometry?, Ballroom B 03 Cross-linking Mass Spectrometry: Basic Strategies and Biological Applications, Room 201 ABC 04 Forensic Mass Spectral Technology: The Transition from Research to Practical Application, Room 204 ABC 05 Advances in High Throughput Sample Preparation for Quantitative Mass Spectrometry-based Studies, Room 102 AB 06 Analysis of High MW Polymers, Room 103 ABC 07 Diversity & Inclusion Committee, Room 104 AB 08 MS Career Options: How to Kick Start Your Career, Room 108 AB 09 Single-Cell Proteomics: From Sample Preparation to Data Analysis, Room 109 AB 10 Teaching Mass Spectrometry: What are the Essential Skills and Concepts that Students Need to Learn at the Undergraduate Level?, Room 110 AB 11 Visualization of Mass Spectrometry Related Data, Room 111 AB 12 Enhancing Environmental Applications with Tandem Ion Mobility Mass Spectrometry, Room 113 ABC 13 Top-down Mass Spectrometry Data Visualization and Identification Using TopMSV, Room 114 **CORPORATE DINNER SEMINARS,** Convention Center (see page 16 for details) 7:00 PM



Consult online planner or mobile app for detailed program. Also includes content for in-person and remote posters.



	ICLODAT
<b>7:00</b> AM	CORPORATE BREAKFAST SEMINARS, Convention Center (see page 16 for details)
7:30 ам - 5:00 рм	REGISTRATION, Grand Hall
8:30 - 10:30 am	ORAL SESSIONS TOA am Imaging: Instrumentation & Method Development; <i>Ballroom A</i> TOB am Structural Biology; <i>Ballroom B</i> TOC am Drug Target Identification by MS; <i>201 ABC</i> TOD am Informatics: Innovations; <i>204 ABC</i> TOE am Lipidomics: Targeted and Untargeted; <i>103 ABC</i> TOF am Fundamentals: Formation and Detection of Big Ions; <i>108 AB</i> TOG am Small Molecules: Quantitative Analysis; <i>113 ABC</i> TOH am Forensics: Innovations and Applications; <i>Room 114</i>
10:30 ам - 2:30 рм	Poster Session and Exhibits, Tuesday Posters, Hall AB Odd-number posters present: 10:30 - 11:30 am PLUS 12:30 – 2:30 pm Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm
2:30 - 4:30 рм	ORAL SESSIONS TOA pm Instrumentation: Innovative Separations Approaches Coupled to MS; <i>Ballroom A</i> TOB pm Biotherapeutics: Proteins, Antibodies, and Antibody/Drug Conjugates; <i>Ballroom B</i> TOC pm Single Cell Omics; <i>201 ABC</i> TOD pm Imaging: Pharmaceuticals, Metabolites, and Lipids; <i>204 ABC</i> TOE pm Protein-Ligand and Protein-Protein Interactions; <i>103 ABC</i> TOF pm Fundamentals: Ion Structures and Energetics; <i>108 AB</i> TOG pm High Throughput MS; <i>113 ABC</i> TOH pm Synthetic Polymers; <i>Room 114</i>
4:45 - 5:30 рм	Award Lecture, Ballroom B Biemann Medal Nuno Bandeira University of California – San Diego
5:45 - 7:00 рм	<ul> <li>WORKSHOPS There are light refreshments in foyers, 5:30 - 5:45 pm.</li> <li>01 Top Down Proteomics and Top Down Mass Spectrometry: Emerging Technologies, <i>Ballroom A</i></li> <li>02 HDX, Covalent Labeling &amp; Cross-Linking: New developments and Applications, <i>Ballroom B</i></li> <li>03 Recent Advances in Oligonucleotides &amp; Peptides Bioanalysis by Triple Quad and HRMS, <i>Room 201 ABC</i></li> <li>04 Bridging Native-MS in Academia and Industry: Nucleic Acids and Their Delivery Systems, <i>Room 204 ABC</i></li> <li>05 The NIH and NSF Review and Funding Process, <i>Room 102 AB</i></li> <li>06 Big Data: Analytics and Metadata for Energy, Petroleum and Biofuels, <i>Room 103 ABC</i></li> <li>07 Quality Control for Proteomics and Metabolomics, <i>Room 104 AB</i></li> <li>08 New Horizons in the Application of Mass Spectrometry in Extractables and Leachables, <i>Room 108 AB</i></li> <li>09 Allyship: Embracing Diversity and Inclusion in Your Workplace, <i>Room 110 AB</i></li> <li>11 Emerging Technologies Advancing Mass Spectrometry Research: 3D Printing, <i>Room 111 AB</i></li> <li>12 Big Particles - Practical Aspects to Trapping Ultra High Masses, <i>Room 113 ABC</i></li> <li>13 Probability-based Metabolite Identification Confidence: How Can We Get There?, <i>Room 114</i></li> <li>14 Achieving Harmonized Clinical Laboratory Testing: Current Best Practices &amp; Future Approaches, <i>Room 105 AB</i></li> </ul>
7:00 рм	Corporate Dinner Seminars, Convention Center (see page 16 for details)
<u> </u>	1





Consult online planner or mobile app for detailed program. Also includes content for in-person and remote posters.



#### WEDNESDAY 7:00 AM **CORPORATE BREAKFAST SEMINARS,** Convention Center (see page 16 for details) 7:30 AM - 5:00 PM **REGISTRATION, Grand Hall** 8:30 - 10:30 AM **ORAL SESSIONS** WOA am Artificial Intelligence in MS Instrumentation and Applications; Ballroom A WOB pm Glycopeptides and Glycoproteins; Ballroom B WOC am Drug Discovery and Pharmacokinetics; 201 ABC WOD am Informatics: Metabolomics; 204 ABC WOE am Nucleic Acids and Oligonucleotides; 103 ABC WOF am Fundamentals: Ion Activation and Dissociation; 108 AB WOG am Antidoping, Cannabis, and Opioid Detection; 113 ABC WOH am Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, and Supplements; Room 114 10:30 AM - 2:30 PM POSTER SESSION AND EXHIBITS, Wednesday Posters, Hall AB Odd-number posters present: 10:30 - 11:30 am PLUS 12:30 - 2:30 pm Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm 2:30 - 4:30 PM **ORAL SESSIONS** WOA pm Instrumentation: New Hybrid and Multimodal Approaches; Ballroom A WOB pm Post-translational Modifications: Qualitative & Quantitative Analysis; Ballroom B WOC pm Metabolomics: New Technologies and Applications; 201 ABC WOD pm Informatics: Peptide and Protein Identification, Proteomics; 204 ABC WOE pm Covalent Labeling and Chemical Crosslinking; 103 ABC WOF pm Challenges in MS Analysis of Complex Mixtures; 108 AB WOG pm Microbiome and Interactome; 113 ABC WOH pm Stable Isotope Labeling: Applications; Room 114 4:45 - 5:30 рм ASMS MEETING, Ballroom B. Awards, board reports, wine, beer, soft drinks - and more! 5:45 - 7:00 PM **WORKSHOPS** There are light refreshments in the foyers, 5:30 - 5:45 pm. 01 From Theory to Revolutionary Instrumentation: Nothing is More Practical than a Good Theory?, Ballroom A 02 Ambient MS and Direct to MS: Strategies for Quantitation, Ballroom B 03 Interpreting Imaging MS Data at 'Omics Level: Integration with Other Omics Platforms, Room 201 ABC 04 Ion Mobility MS Data Analysis Tools: What's There and What Isn't, Room 204 ABC 05 The International Metaproteomics Initiative: Communicating and Advancing Metaproteomics Research, Room 102 AB 06 MS Libraries for Compound Identification, Room 103 ABC 07 Developing World Outreach, Room 104 AB 08 Networking for Scientists: Celebrating Women Mass Spectrometrists, Room 108 AB 09 New Aspects in the Development of Multi-Attribute Method (MAM), Room 109 AB 10 LC-MS for Translational DMPK and Precision Medicine, Room 110 AB 11 Real-time Mass Spectrometry in Proteomics and Beyond, Room 111 AB 12 Protips and Life Hacks for FTMS. Room 113 ABC 13 Trans-Proteomic Pipeline: Recent Advances and Future Directions, Room 114 14 Utilization of Mass Spectrometry in Cannabis & Hemp Analysis, Room 105 AB 15 Metabolomic Applications in Human Health and Environmental Sciences, Room 107 B 7:00 рм **CORPORATE DINNER SEMINARS,** Convention Center (see page 16 for details)



Consult online planner or mobile app for detailed program. Also includes content for in-person and remote posters.

# **PROGRAM OVERVIEW**



INORSDAT		
<b>7:00</b> AM	CORPORATE BREAKFAST SEMINARS, Convention Center (see page 16 for details)	
7:30 ам - 5:00 рм	REGISTRATION, Grand Hall	
8:30 - 10:30 am	<b>ORAL SESSIONS</b> ThOA am Instrumentation: Innovations in High-Resolution Mass Spectrometry; <i>Ballroom A</i> ThOB am Biomarkers: Qualitative Analysis; <i>Ballroom B</i> ThOC am Drug Discovery and Development : Quantitative Analysis; <i>201 ABC</i> ThOD am Informatics: Multiomics Integration and Applications; <i>204 ABC</i> ThOE am Lipidomics: New MS Technologies and Applications; <i>103 ABC</i> ThOF am Fundamentals: Ion-Molecule, Ion-Ion, Ion-Electron Reactions; <i>108 AB</i> ThOG am Environmental: Non-Target Analysis and Emerging Contaminants; <i>113 ABC</i> ThOH am H/D Exchange: Innovations and Applications; <i>Room 114</i>	
10:30 ам - 2:30 рм	Poster Session and Exhibits, Thursday Posters, Hall AB Odd-number posters present: 10:30 - 11:30 am PLUS 12:30 – 2:30 pm Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm	
2:30 - 4:30 рм	ORAL SESSIONS ThOA pm Instrumentation: New Developments in Ionization and Sampling; Ballroom A ThOB pm Biomarkers: Quantitative Analysis; Ballroom B ThOC pm Clinical Analysis: Applications; 201 ABC ThOD pm Ion Mobility: Structure Determination; 204 ABC ThOE pm Quantitative Proteomics in Systems Biology; 103 ABC ThOF pm Fundamentals of Ionization; 108 AB ThOG pm Natural Product Discovery and Biotechnology; 113 ABC ThOH pm Exposomics, Toxicology, and Health Outcomes; Room 114	
4:45 - 5:30 рм	PLENARY LECTURE, Ballroom B         Computer Vision and the Neural Network Revolution         William T. Freeman         Massachusetts Institute of Technology	
5:30 - 7:30 рм	FAREWELL TOAST & RECEPTION, Poster-Exhibit Hall Sponsored by Shimadzu Scientific Instruments	

# THURSDAY







In-Person Poster Presentation Schedule Odd-number posters present: 10:30 am - 11:30 am PLUS 12:30 – 2:30 pm Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm

#### **IN-PERSON MONDAY POSTERS**

Set up all Monday posters 7:00 - 8:00 am

Odd-numbered posters present 10:30 - 11:30 am PLUS 12:30 - 2:30 pm

10.30 - 11.30 anti E03 12.30 - 2.30 pr

Even-numbered posters present 10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

> Remove all Monday posters 7:00 - 8:00 pm

Art, Archaeology & Paleontology	001
Big Ion MS	002-005
Biomarkers: Quantitative Analysis	006-027
Data-Dependent Acquisition	028-047
Disease Biomarkers	048-060
Epigenetic Modifications	061-068
Food Safety & Chemistry: Foodomics, Allergens,	
Bacteria, Foods, and Supplements	069-086
Food Safety: General	087-106
Fundamentals: Formation and Detection	
of Big lons	107-120
Fundamentals: Ion Molecule, Ion/Ion,	
Ion/Electron Interactions	121-129
Fundamentals: Ion Spectroscopy	130-135
Fundamentals: Ion Structure/Energetics	136-139
Fundamentals: Ionic Clusters	140-141
Fundamentals: Ionization	142-146
Fundamentals: Metal Ion Cationization,	
Metal-Ligand Interactions, Catalysis	147-149
Fundamentals: Molecular Modeling/Quantum	
Mechanical Calculations	150-151
Fundamentals: Native MS	152-155
Fundamentals: Photodissociation	156-157
Imaging MS: Computational Methods, Software,	
and Analysis	158-171
Informatics: Algorithms and Statistical Advances .	172-189
Informatics: General, SRM, and DIA	190-192
Instrumentation: General	193-203
Ion Mobility: Fundamentals	204-207
Ion Mobility: General	208-222
Lipids: General	223-241
Metabolomics: Clinical Applications	242-254
Microorganisms and the Microbiome	255-268
Nanomaterials	269-270
Nanoscale and Microfluidic Separations and MS .	271-274
Phosphopeptides: Enrichment Methods	275-290
Plants: Systems, Biotechnology, and	
Natural Products	291-301
Polymers	302-308
Process Development MS	309-316
Protein Therapeutics: Quantitative Analysis	317-332
Proteins: Conformation Analysis and Structural	
Biology	333-347
Proteomics: Quantitative	348-390

#### **IN-PERSON POSTERS**

Set up all Tuesday posters 7:00 - 8:00 am

**Odd-numbered posters present** 10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present 10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Tuesday posters

7:00 - 8:00 pm

Biomarkers: Discovery	001-035
Biomolecular Structure Analysis: Chemical	
Crosslinking and Covalent Labeling	036-064
Clinical Analysis	065-093
Environmental: General	094-132
Glycoproteins	133-173
Imaging MS: Method Development	174-194
Informatics: Metabolomics	195-200
Informatics: Multiomics Integration	201-209
Ion Mobility: FAIMS/DMS	210-223
Lipids: Profile Analysis	224-239
MALDI: Applications	240-247
MALDI: Innovations in Instrumentation	248-250
MALDI: Sample Preparation	251
Metabolomics: Identification of Unknown	
Metabolites	252-261
Metabolomics: Sample Preparation	262-268
Natural Products	269-274
Peptidomics	275-289
Protein Therapeutics: Structural	
Characterization	290-310
Proteins: PTMs	.311-329
Proteomics: Infectious Diseases	330-347
Proteomics: Intact Proteins	348-350
Proteomics: Top Down Analysis	351-374
Proteomics: Top Down Analysis	375-380
Toxicology	381-387

Poster numbers shown for topics are guideline only. Consult mobile app for up-to-date poster numbers by topic.

Con app incl and

Consult online planner or mobile app for detailed program. Also includes content for in-person and remote posters.



**REMOTE POSTER CONTENT** is included in the mobile app and online planner.



#### **POSTER OVERVIEW**



In-Person Poster Presentation Schedule Odd-number posters present: 10:30 am - 11:30 am PLUS 12:30 – 2:30 pm Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm

#### **IN-PERSON WEDNESDAY POSTERS**

Set up all Wednesday posters 7:00 - 8:00 am

**Odd-numbered posters present** 10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present

10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Wednesday posters 7:00 - 8:00 pm

Ambient Ionization: Applications	001-015
Ambient Ionization: Fundamentals and	
Instrumentation	016-033
Cannabis	034-052
Education: Teaching MS and Teaching with MS	053-055
Elemental Analysis: ICP/MS	056-059
Energy: Biofuels and Algae	060-061
Energy: Petroleum and Biofuels	062-068
Environmental: Exposomics	069-071
Environmental: Pharmaceuticals and Pesticides	072-082
Exposomics	083-085
GC/MS: General	086-089
GC/MS: Instrumentation and Applications	090-100
Homeland Security	101
Imaging MS: Disease Markers	.102-118
Informatics: Peptide ID and Quantification	.119-136
Instrumentation: New Developments in	
Ion Detection	137-139
Instrumentation: New Developments in	
Ionization and Sampling	140-165
Instrumentation: New Developments in	
Mass Analyzers	166-173
Ion Mobility: Applications	174-203
Isotope Labeling and Fluxomics Applications	204-208
LC/MS: Chromatography and Software	209-218
LC/MS: General	219-227
Lipids: ID and Structural Analysis	228-242
Metabolomics: Targeted and Quantitative	
Analysis	243-257
Peptides: Fragmentation Mechanisms	258
Peptides: PTM Identification	259-276
Peptides: Sequence Analysis	277-279
Proteins: General and Membrane	280-291
Proteomics: Clinical Applications	292-312
Proteomics: New Approaches	313-343
Single Cell MS	344-357
Small Molecules: Quantitative Analysis	358-380

#### **IN-PERSON THURSDAY POSTERS**

Set up all Thursday posters 7:00 - 8:00 am

**Odd-numbered posters present** 10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present 10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

> Remove all Thursday posters 7:00 - 8:00 pm

Antibodies & Antibody Drug Conjugates Carbohydrates Drug Discovery/DMPK/ADME Drug Metabolism: Qualitative Analysis Drug and Metabolite Analysis Forensics H/D Exchange: Hardware, Software and	001-017 018-042 043-053 054-059 060-076 077-101
Methodology	. 102-111
H/D Exchange: Protein Structure/Function	.112-130
High Mass Accuracy/High Performance MS:	
Applications and Instrumentation	131-139
Imaging MS: Pharmaceuticals, Metabolites,	
and Lipids	140-163
Informatics: Workflow and Data Management	164-176
Instrumentation: Mini/Portable/Fieldable MS	178-185
Instrumentation: New Concepts	186-194
Ion Mobility: Structure	195-204
LC/MS: Sample Preparation	205-225
Lipids: Targeted and Quantitative Analysis	226-238
Metabolomics: Untargeted Metabolite Profiling	239-262
Nucleic Acids and Oligonucleotides	263-289
Peptides: Targeted and Quantitative Analysis	290-306
Proteins: Complexes/Non-covalent Interactions	307-324
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Poster numbers shown for topics are guideline only. Consult mobile app for up-to-date poster numbers by topic.



Consult online planner or mobile app for detailed program. Also includes content for in-person and remote posters.



**REMOTE POSTER CONTENT** is included in the mobile app and online planner.





#### **MONDAY WORKSHOPS**

# 01 Kahoot! Interactive Trivia on LC-MS Related Topics LCMS & Related Topics Interest Group Presiding: Erik Soderblom; James Dodd

### **Ballroom A**

Need a break from formal talks? Already an expert in LC-MS and want to impress your friends? Not an expert and want to learn something about LC-MS? Just like interactive trivia games where you compete against a room of like-minded people? Well, this workshop is for you! Kahoots! is a real-time trivia based game in which you use your personal handheld devices (phone/tablet) to answer fun trivia questions. Anonymized attendee's points are updated in real time and displayed for the entire audience after each guestion - the race is on! Although the Kahoot! board has been refreshed from ASMS 2019, the LC-MS and Related Topics Interest Group Workshop will remain focused on various aspects of Proteomics, Pharmacokinetics, Metabolomics, Laboratory Automation, and Increasing Sample Throughput. Following each question, audience-driven comments/thoughts/considerations will be encouraged. Will it be Yellow Goat. Skunky Salamander. or YOU that takes home the grand prize this year - come and find out at LC-MS Kahoots!

#### 02 Machine Learning: How Is It Enhancing **Mass Spectrometry?** Presiding: Gaurav Chopra **Ballroom B**

Recent advances in machine learning and artificial intelligence (AI) are revolutionizing the human/technology interface. Mass spectrometry (MS) is a powerful analytical tool that is extensively used for characterization of substances and mixtures across many fields, such as chemistry, biology, pharmaceuticals, petroleum, etc. Machine learning tools are emerging to support autonomous science, in which critical decision-making on experimental design is conducted by algorithms rather than by human intervention. This shift from automation to autonomation is enabled by rapid advances in data science and deep neural networks. We will discuss several guestions with selected 5 minutes of overview presented by experts in the field: How machine learning/AI algorithms is enhancing MS autonomation? Does machine learning/AI enhance analysis of ionmolecule reactions, ion-ion reactions, multiple reaction monitoring, nano-DESI, proteomics, metabolomics, lipidomics, etc.? How does chemical representation affect MS analysis and results? What are the current challenges in MS methods that machine learning/AI can and cannot address? Is it possible to develop an autonomous methodology that can be easily implemented into commercial mass spectrometers with only minor instrument modifications? Can we develop machine learning methods that are understandable by human chemists for decision making? Are there specific deep learning architectures that work better than others for identifying structure from spectra? Do we need MS scientists trained in data science to handle the exponential increase in data obtained using mass spectrometry? Our workshop will address revolutionary changes in data science and artificial intelligence that may result in new opportunities at the interface between data and MS based measurement science.

#### 03 Cross-linking Mass Spectrometry: Basic Strategies and Biological Applications Presiding: Lan Huang Room 201 ABC

Cross-linking mass spectrometry (XL-MS) is a powerful and emergent technology for interactomics and structural proteomics. In comparison with other MS-based structural tools. XL-MS is unique owing to its capability of simultaneously capturing protein-protein interactions (PPIs) from their native environments and uncovering interaction contacts, thus permitting the determination of both identity and connectivity of PPIs in cells. The identified crosslinks can be used to generate protein interaction networks and to elucidate architectures of protein complexes through computational modeling. Recent advancements of XL-MS technologies have made experimental workflows reliable and robust for systems-wide analysis. The availability of cross-linking reagents, instrumentation and software enables XL-MS experiments accessible to a broad research community. This workshop will serve as an educational forum to cover various aspects of XL-MS technologies. experimental strategies, data analysis and biological applications in protein structural analysis. In addition, current status and future perspectives will be presented to benefit both newcomers and experienced researchers. Ample time will be allocated for guestions and answers including an opportunity for novices/students to contribute anonymous questions on fundamentals.

#### 04 Forensic Mass Spectral Technology: The Transition from Research to Practical Application Forensics & Homeland Security Interest Group Presiding: Brittany Casey; Ruth Smith Room 204 ABC

The use of mass spectrometry in forensics and homeland security is constantly evolving to improve analyte detection and identification in some of the most difficult matrices and, in the field of homeland security, often in suboptimal settings. As the reliability of results obtained in these situations is critical, methodologies and technologies are constantly being updated and modernized primarily through academic research. However, the transition of such new methodologies and technologies from the academic research lab to practitioners is challenging and can be a lengthy, complicated process due to high costs and lack of instrumentation and training. Open communication between academicians and practitioners is essential to facilitate this transition and benefit each party.

This year the workshop will again highlight mass spectrometry applications across diverse subsections within the fields of forensics and homeland security. A panel of representatives from academic, private, and government laboratories will discuss the development of new applications of mass spectrometry and the analytical needs in the forensic laboratory. Participants will gain insight into the implementation challenges faced by practitioners and the practical factors that limit the adoption and operation of new technologies and methodologies in forensic laboratories.



#### **MONDAY WORKSHOPS**

# 05 Advances in High Throughput Sample Preparation for Quantitative Mass Spectrometry-based Studies Presiding: Pankaj Dwivedi

Room 102 AB

The field of quantitative proteomics and metabolomics is moving towards high throughput-based automated sample preparation, this workshop will provide a platform to discuss new advances as well as development in this field.

The major sections which will be discussed in this workshop are as follows:

(1) How does proteomics and metabolomics sample preparation affect the overall MS data quality?

(2) What are new advances in sample preparation using automation?

(3) Advantages and disadvantages of automated sample preparation (high throughput) compared to the traditional low throughput workflows.

(4) Recent developments in the field of TMT based quantitative proteomics.

Presentation Topics include:

- Quantitative Proteomics in Low Volume Samples; Bhagwat Prasad (Washington State University)
- Multiplicative increase in the sensitivity and throughput of data independent acquisition; Nikolai Slavov (Northeastern University)
- Enabling large-scale proteomics studies through parallelization, automatization and quality management; Christoph Messner (Biognosys)
- TMT isobaric labeling and real-time search MS 3 methodologies for proteome quantitative analysis; Qin Fu (Cornell University)
- Serum metabolomics analysis reveals novel biomarkers and pathways for effectiveness of Benfotiamine in Alzheimer's disease; Ruchika Bhawal (Cornell University)

#### 06 Analysis of High MW Polymers Polymeric Materials Interest Group Presiding: Jessica Hoskins; Thierry Fouquet Room 103 ABC

This year's meeting will consist of three distinct sections: a workshop, poster elevator-talks, and an open forum. To begin, we will have a short tutorial session on mass spectrometry of large (>>10 kDa) polymers. This topic was chosen based on feedback from last year's polymeric materials workshop participants and will be structured to encourage interactive discussion within the group.

Second, we will host an open series of short (3-5 min each) promotions of polymer related posters by any presenters who wish to highlight their work to the workshop's specialized audience.

The workshop will conclude with an open forum in which attendees are invited to bring up any polymer-related issues or questions that they would like help with. In addition, input will be sought for future Polymer Workshop topics.

#### 07 Building and Implementing Effective DEI Initiatives in the Laboratory Space

Presiding: ASMS Diversity and Inclusion Committee: Candice Ulmer (Chair), Jennifer Campbell, Saiful Chowdhury, Dominic Gostick, Carlos Larriba Andaluz, Richard Yost (ASMS Board Rep.)

#### Room 104 AB

Recently, we've witnessed academic institutions, industries, and government agencies actively striving to create a supportive, diverse, equitable, and inclusive environment for laboratorians. However, despite these grand efforts, many scientific organizations, laboratory groups, and workplaces still struggle with recognizing implicit bias and microaggressions, recruiting/ retaining students and employees, designing effective DEI training tools, and implementing corrective actions for issues encountered. Nevertheless, laboratory environments do exist where scientists are encouraged to be supportive, inclusive, and appreciative of diversity, which has resulted in their increased productivity, creative innovations, and varied perspectives while developing solutions to complex problems. As a result, topics discussed during this workshop will include effective and noneffective strategies for implementing DEI in the workplace, implications of a lack of diversity, allyship, and much more. Attendees will participate in a facilitated discussion by a panel of speakers leading the DEI effort in various laboratories and academic institutions. This interactive workshop is designed to provoke discussion from laboratorians in all sectors of the workforce, including undergraduate and graduate students.

#### 08 MS Career Options: How to Kick Start Your Career Young Mass Spectrometrists Interest Group Presiding: Laura Sanchez; Christopher Rose Room 108 AB

The Young Mass Spectrometrists workshop focuses on a panel discussion where representatives of various careers paths discuss their journey to their current position and answer questions regarding their current and past experiences. Through this discussion mass spectrometrists at the undergrad, graduate, or postdoctoral stage of their career learn information or strategies that will help them navigate the next steps in their career. This panel typically comprises representatives from academia, biotech/pharma, start-up companies, government, and non-traditional career paths to provide a comprehensive view of career opportunities for young researches who have mass spectrometry skills. In addition to a large group discussion with the panel - we will also have breakout groups where attendees will have the ability to interact with the representative of their choosing in a smaller group format.

#### 09 Single-Cell Proteomics: From Sample Preparation to Data Analysis Presiding: Ying Zhu; Ryan Kelly Room 109 AB

There is growing interest in extending LC-MS-based bottom-up proteomics analysis to single cells. Single-cell proteomics can reveal critical insights on biological systems that are masked in bulk-scale proteomics, including diverse cell populations and subpopulations, cell developmental trajectories, and tissue microenvironments. However, because of the orders-of-magnitude reduction in sample input for single cells relative to bulk-scale proteomics, the comprehensive characterization of the singlecell proteome is still immature and confronts many technical



#### **MONDAY WORKSHOPS**

challenges. These challenges include but are not limited to cell isolation, sample preparation, LC separation, MS measurement, data analysis and visualization. As such, all procedures must be carefully optimized and new technologies are needed to advance this field.

In realizing these challenges and great opportunities, we propose to organize the single-cell proteomics workshop. There are three main aims: (1) We will invite the leading scientists to provide an update of technology advances and biological applications in the field; (2) These talks will also serve as tutorials with the aim to reduce technical barriers and to disseminate the developed technologies; (3) We will discuss and summarize the remaining technical challenges and encourages more scientists to join this field. At the end of the workshop, we will hold a roundtable discussion among panelists to answer the questions from attendees, and discuss the formation of a single-cell proteomics interest group to promote collaborations.

#### Presenter/Panelists:

Alexey I. Nesvizhskii (University of Michigan), Jennifer Van Eyk (Cedars-Sinai Medical Center), Yiran Liang (Brigham Young University), and Nikolai Slavov (Northeastern University)

#### 10 Teaching Mass Spectrometry: What are the Essential Skills and Concepts that Students Need to Learn at the Undergraduate Level? Undergraduate Research in MS Interest Group Presiding: Matt Joyner Room 110 AB

Teaching mass spectrometry to undergraduates can be a challenging task. There is often not a single, dedicated course devoted to teaching mass spectrometry at the undergraduate level, leaving instructors the task of integrating essential training related to mass spectrometry in different courses at different institutions. Research in chemical education indicates that helping students differentiate between concepts and skills can significantly enhance student learning. Research in educational psychology also shows that experts often perform many non-obvious or hidden steps when problem solving that can be difficult for the expert to explain and even more difficult for students to learn. In this workshop, we will utilize the shared experience and wisdom of workshop participants to identify essential concepts and skills needed for teaching mass spectrometry to undergraduate students. Participants will also have the opportunity to share pedagogical approaches that enhance student learning. This workshop will be designed to be highly interactive and incorporate input from participants to generate practically useful guidance for enhancing teaching of mass spectrometry at the undergraduate level.

#### 11 Visualization of Mass Spectrometry Related Data Bioinformatics MS Interest Group Presiding: Arzu Tugce Guler; Claire O'Donovan Room 111 AB

Data visualization is an effective way of exploring and presenting complex mass spectrometry data. Visualization is essential not only for quality checks and observation of trends, but also for quick and clear communication of findings from the data. Almost all vendor analysis software come with data visualization capabilities and many third party analysis tools support visualization of mass spectrometry data in native vendor format and/or in one of the open data formats. It is usually possible with these software to visualize the results of the data analysis well, for instance as heat maps and volcano plots. With the wider applicability of mass spectrometry in different fields and experimental setups, external visualization tools and packages are also being used to add or highlight relevant information on top of conventional MS data visualizations. This workshop will focus on conventional and sophisticated visualization techniques and tools for mass spectrometry related data. We will give some up-to-date, concrete examples from mass spectrometry-based proteomics and metabolomics. We aim this workshop to be interactive, so that the attendees can brainstorm what kind of techniques and tools they could use for their own data while conforming to good data visualization practices.

#### 12 Enhancing Environmental Applications with Tandem Ion Mobility Mass Spectrometry Environmental Applications Interest Group Presiding: Andrew Ottens; Paul Chiarelli; Pierangela Palma Room 113 ABC

A recent proliferation of commercial tandem ion mobility mass spectrometers has sparked growth in their application to environmental analyses. Collision cross section measures provide complementary selectivity to resolve complex mixtures and aid in species differentiation and identification. This workshop will explore the introduction of ion mobility into environmental MS analyses across varied sectors from isomeric differentiation of pollutants in drinking water, structural characterization of oil fractions, to providing wider analyte coverage in environmental health outcomes research. The topic will be introduced through data-blitz presentations by early-career scientists to be followed by a discussion led by panelists with relevant expertise. A primary goal is to stimulate thoughts and share recent experience implementing ion mobility into analytical workflows. Additional points of discussion are likely to include libraries for collisional cross section data, software for handling ion mobility data, and other issues relevant to the wider implementation of the technology in environmental MS fields.

#### 13 Top-down Mass Spectrometry Data Visualization and Identification Using TopMSV Presiding: Xiaowen (Kevin) Liu; Liangliang Sun; Si Wu Room 114

#### **Room 114** Top-down mass spectrometry (MS) has gained increasing attention in the past decade because of its capability to sequence whole proteoforms with post-translational modifications (PTMs) and other alterations. Although many computational methods have been developed for top-down MS data analysis, it is still challenging for MS labs to efficiently identify and quantify proteoforms because of the complexity of the data and methods. TopMSV is a webbased tool for top-down MS data processing and visualization. It integrates software tools for spectral deconvolution and proteoform identification and uses analysis results of the tools to annotate topdown MS data. It provides various 2D and 3D views for top-down MS data visualization. Researchers can use TopMSV to quickly explore LC profiles, LC-MS maps, MS and MS/MS spectra, and spectral deconvolution and proteoform identification results. We will give tutorials on TopMSV and TopPIC suite for proteoform identification and guantification as well as the application of the tools to various research problems. We will discuss with users and collect their feedback and suggestions for further improvement of

the tools.



#### **TUESDAY WORKSHOPS**

#### 01 Top Down Proteomics and Top Down Mass Spectrometry: Emerging Technologies Top-Down Proteomics Interest Group

# Presiding: Joe Cannon; Caroline DeHart; Frederik Lermyte Ballroom A

Top down (TD) protein mass spectrometry (MS), when performed optimally, provides unique information that is not accessible with more sensitive bottom up methods. While conceptually simple, there are technical challenges that must be overcome to perform a successful TD experiment or analysis. In this workshop, we will invite experts in industry and academia to showcase new technological advances from separations to MS to bioinformatics that broaden the utility of TD-MS and TD proteomics. There will be emphasis on educating the greater community on new capabilities in the field that increase sensitivity, throughput, and the amount of information achievable. We will focus on new separation technologies that are used for intact protein analysis, on MS advances that facilitate more quantitative or informative analyses, on new computational approaches, and finally on the application of some of those new technologies. Each topic will be introduced by a short presentation, followed by audience discussion and debate. Please contact workshop chairs if you are interested in presenting an introduction to spark the discussion of a topic.

#### 02 HDX, Covalent Labeling & Cross-Linking: New developments and Applications HDX Covalent Labeling & Cross Linking Interest Group Presiding: Miklos Guttman; Fabio Gozzo; Corie Ralston Ballroom B

Developments in MS instrumentation, sample preparation strategies, reagents and informatics tools have significantly advanced applications of HDX, covalent labeling and crosslinking approaches in protein structural and interaction analysis. This workshop will feature invited speakers with expertise in HDX, chemical labeling, and cross-linking methods to introduce each methodology, discuss ongoing developments, highlight any strengths and limitations, and point out things to see while at ASMS related to these methods. The second part of the workshop will focus on exciting new technical developments within HDX/XL/CL-MS through 5 min talks from invited members of the community. The speakers will form a panel for the last portion of the workshop to address questions including an opportunity for novices/students to contribute anonymous questions on fundamentals. One of the organizers will oversee the online portion of the workshop to support the 'hybrid' format of the meeting this year.

#### 03 Recent Advances in Oligonucleotides & Peptides Bioanalysis by Triple Quad and HRMS Regulated Bioanalysis Interest Group Presiding: Jian Wang; Dian Su Room 201 ABC

There were nine oligonucleotide and fourteen peptide drugs approved by Food and Drug Administration (FDA) from 2016 to 2020. Particularly with the recent approval of two oligonucleotide and four peptide (one antibody-drug conjugate) therapeutics in 2020, we are looking forward to seeing expanded interests in medium-size therapeutics. The 2021 ASMS Regulated Bioanalysis Interest Group (RBIG) Workshop is focused on "Recent Advances in Oligonucleotides & Peptides Bioanalysis by Triple Quad and HRMS". We would like to build our discussion on the conclusions and recommendations from the 2018 White Paper in Bioanalysis: https://www.future-science.com/doi/pdf/10.4155/bio-2018-0268

#### Oligonucleotides

"...LC-MS/MS and HRMS analysis, selection of an IS that matches chemistry and stereochemistry (if necessary)with the aim to obtain the same extraction efficiency as the analyte, is challenging; To increase sensitivity, double liquid-liquid extractions using phenol and chloroform combination or SPE, IA enrichment, or selecting multiple target ions are options but should be carefully evaluated;..."

#### Peptides

"The use of quantitative HRMS over unit resolution MS is analyte and matrix dependent. One option to improve sensitivity for therapeutic peptides analysis can be to sum multiple MRM as long as specificity/selectivity has been carefully evaluated; the signal to noise ratio needs to increase when summing multiple transitions;..."

This workshop will develop future discussions and consensus on Regulated Bioanalysis of oligonucleotides & peptides including topics on sample preparation, Mass Spectrometric methods and data processing. Experts in the field will share their experience in this highly interactive workshop.

#### 04 Bridging Native-MS in Academia and Industry: Nucleic Acids and Their Delivery Systems Native Mass Spectrometry Interest Group Presiding: Michael Marty; Iain Campuzano; Elizabeth Hecht Room 204 ABC

Since the initial experiments performed in academia demonstrating the retention of noncovalent protein-ligand and protein-protein complexes in the gas-phase, native MS has grown into a fully established research field. This unique area has given rise to the development of specialized MS hardware for the transmission and detection of ultra-large ions and methods allowing characterization of complex and emerging pharma modalities and new research targets.

Interest in the therapeutic use of nucleic acids in a variety of forms has grown significantly since its first clinical trials in the early 1990s. The recent unprecedented advances in mRNA vaccines represents the success of one class of nt. based drugs that also includes siRNA, nucleic acid conjugates, and aptamers.

Although native MS has most commonly been employed to study protein complexes, a small community has driven significant advances in native MS of nucleic acids. Beyond the nucleic acids themselves, the delivery vehicle can be critical to the success of nucleic acid therapeutics. A wide range of potential delivery options are available, ranging from antibody conjugates, lipid nanoparticles, polymer networks/gels, or viral capsids. Native mass spectrometry is uniquely suited to characterize these complex systems and support research and development for novel nucleic acid therapeutics.

Within this workshop, we will discuss the diversity of nucleic acid-based systems now being studied by native-MS in both academia and pharma and the new technologies for studying these complex systems. Our focus is to bridge new technology and



#### **TUESDAY WORKSHOPS**

applications development in both academic and pharma research environments, allowing for routine project support and progression for modalities that require native MS analytics.

#### 05 The NIH and NSF Review and Funding Process Presiding: Salvatore Sechi; Kelsey Cook; Douglas Sheeley; Kenneth Ryan Room 102 AB

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. Tips on grant writing and insights into the review process will be presented. The session will also provide an opportunity to inquire about the latest initiatives and priorities. 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.

#### 06 Big Data: Analytics and Metadata for Energy, Petroleum and Biofuels Energy Petroleum & Biofuels Interest Group Presiding: Amy McKenna; Leonard Nyadong Room 103 ABC

The burgeoning trend in big data analytics (BDA), which allows speedy and efficient examination of large amounts of data to uncover hidden patterns, correlations and other insights presents a new frontier for energy research. In the case of fossil, biofuels, and other complex organic mixtures (e.g., natural organic matter, emerging contaminants) high resolution mass spectrometrybased approaches play a vital role for detailed molecular-level characterization. However, the ability to uncover information from high resolution mass spectra data sets is being pushed to the limits of instrumentation and methodological capabilities. These analyses often routinely generate over 50,000 peaks in the case of crude oil, which challenges data analyses. Most of the data analytics tools developed for data visualizing, which include Kendrick mass defect and van Krevelen analyses and other statistics analyses are limited to only a few data sets. Big data analytics in the petroleum and biofuels field provides opportunity to uncover novel correlations in the molecular-level analytical measurements to macroscopic behavior to enable enhanced upgrading value. Big data analytics include collecting data from different sources, which can be very challenging in terms of compatibility, using the right data and the right tools to make the right decisions in real time. Several types of tools are often required to work together to collect, process, cleanse, and analyze big data.

This workshop will focus on an open discussion format with panelists to jumpstart conversations on the challenges and enablers for application of big data analytics in the petroleum and biofuels field. The discussions will focus on some of the prerequisites for developing big data analytics capability, which include: (1) Finding the right tools and platforms; (2) Making big data accessible; (3) Maintaining quality data; and (4) Keeping data secure; and (5) Types of metadata required for each sample type. The workshop will consist of short three-four slides by each panelist, followed by an open forum question and answer and discussion.

#### 07 Quality Control for Proteomics and Metabolomics Presiding: David Tabb; Wout Bittremieux Room 104 AB

Throughout biological mass spectrometry, researchers are prioritizing repeatability and reproducibility of experimentation. This workshop, presented by members of the HUPO PSI (Proteomics Standards Initiative) Quality Control Working Group, will demonstrate methods in quality control (QC) and quality assurance for mass spectrometry.

The presentations and discussions will emphasize real-life scenarios, using published experiments as a starting point. The team will demonstrate how to transform a collection of LC-MS/ MS raw data into quality metrics and how to make inferences or decisions based upon these metrics (such as recognizing batch effects and outliers). The mzQC file format created by this team to communicate quality information will be shown in action, enabling software tools from different laboratories to communicate.

Some of the questions we hope to answer with participants include the following: How can QC samples be incorporated in your experimental design? How do different sample processing steps influence the measured data, for example, by inadvertently introducing artificial modifications? Is it possible to disentangle the influence of technical and biological variability? Which user-friendly software tools are available to assess data quality?

#### 08 New Horizons in the Application of Mass Spectrometry in Extractables and Leachables Presiding: Atish Sen; Douglas Kiehl; Stephen Warren

#### Room 108 AB

Mass spectrometry is now integral to the analysis of extractables and leachables in the pharmaceutical, food and environmental industries. Extractables and leachables analysis has now become an essential part of specifications on release, stability and life cycle management for both small molecule and biologics drug products. Regulatory organizations are giving increased scrutiny to E&L with rapidly evolving expectations. Mass spectrometry being an important tool in identifying and assessing E&L compounds originating from packaging, manufacturing and drug delivery systems. This workshop will discuss advances in the use of MS and related techniques for achieving comprehensive characterization and profiling of E&L.

#### 09 Allyship: Embracing Diversity and Inclusion in Your Workplace Career Development Interest Group Presiding: Lucinda Hittle; Troy Wood Room 109 AB

As we look to truly embrace diversity and inclusion in the workplace, developing and strengthening our ability to serve as an ally for others is essential. This interactive workshop will focus on specific workplace scenarios through small group breakout discussions. Participants will have a chance to learn steps to active allyship,



#### **TUESDAY WORKSHOPS**

do's and don'ts, and collectively discuss their challenges and lessons learned. This workshop is designed to bring together mass spectrometrists from all environments including, but not limited to, mass spectrometry vendors, chemical, pharmaceutical, forensic and academic scientists. Attendees will be divided into small groups for break-out discussions. Participants will have the opportunity to rotate through these small group sessions in a "speed dating" format to discuss as many scenarios as possible and enhance networking. Each small group will have an experienced scientist and facilitator. All are welcome.

#### 10 Data Independent Acquisition: From Data Acquisition to Analysis Data Independent Acquisition Interest Group Presiding: Florian Meier; Lindsay Pino

#### Room 110 AB

In recent years, data independent acquisition (DIA) schemes have become increasingly popular as they promise high levels of reproducibility and data completeness in large sample cohorts, suitable for systems biology and translational research.

With advances in the latest generation of mass spectrometers and liquid chromatography systems, the scale of DIA experiments has dramatically increased through the combination of shorter chromatography gradients with the speed of time-of-flight. This is also facilitated by emerging acquisition schemes such as scanning quadrupole-type or ion mobility-enhanced methods. These trends have also fueled the development of faster, more scalable, and user-friendly software, including support for advanced data structures. Larger datasets also come with statistical challenges that have not been fully investigated for label-free quantitative mass spectrometry data, such as normalization, batch effect correction, and significance testing for complex experimental designs.

At the same time, the range of applications for DIA is continuously expanding, for example, to the quantitative analysis of posttranslational modifications beyond phosphorylation, including ubiquitination and acylation. PTM analysis may further benefit from new fragmentation methods. Although some work has been done to expand DIA to other areas of mass spectrometry such as small molecule and imaging proteomics, these approaches have not been fully implemented and are areas of active research.

In this workshop, we invite experts in the field to discuss technological and software innovations, as well as promising biological and medical applications. The open format should engage discussions about unique challenges, but also opportunities for future developments.

#### 11 Emerging Technologies Advancing Mass Spectrometry Research: 3D Printing Presiding: Kristof B. Cank, Herma C. Pierre Room 111 AB

This workshop series will concern the use of auxiliary technologies that support advancements in the field of MS. 3D printers allow for quick prototyping this quickly finding their way into laboratories. Discussion at the workshop will focus on the implementation of 3D printing to support MS research.

# 12 Big Particles - Practical Aspects to Trapping Ultra High Masses

#### Ion Trap MS Interest Group Presiding: Theresa Evans-Nguyen; Dalton Snyder Room 113 ABC

Extending the mass range of ion traps to large particles such as virions and protein complexes seems particularly relevant in the age of COVID. At first glance, the shift in application of ion traps to high mass analysis requires a simple shift to lower frequency fundamental waveforms. However, nuances of space-charge repulsion, collision cross-section, electronic instrumentation control, and detection methods are worth consideration. We will invite a panel of prominent researchers in the field to lavout the current state of the art in ultra-high mass analysis by ion traps. Presentations will be solicited to identify the practical aspects and major challenges of using traps to explore the high mass regime. Following these presentations, we will open discussion to such topics as orthogonal technologies in spectroscopy, intersectional interest with aerosols, and bio-particle application needs. By focusing the use of ion traps explicitly on large particle analysis, we hope to foster wider interest, crowd-source new ideas, and encourage greater community and collaboration.

#### **13 Probability-based Metabolite Identification Confidence: How Can We Get There?** Presiding: Thomas Metz; Oliver Fiehn; Gary Patti

#### Room 114

In metabolomics studies, the determination of confidence in metabolite identifications is ultimately made by individual researchers. After applying tolerance thresholds for e.g. mass accuracy or MS/MS library scores, researchers manually perform comparisons and annotations, accepting or rejecting the results based on arbitrary or subjective criteria. The Chemical Analysis Working Group of the Metabolomics Standards Initiative (MSI) published in 2007 the first proposed minimum reporting standards for metabolite identification confidence, which consisted of four MSI-levels of confidence in decreasing order based on the amount and degree of orthogonality of the analytical information supporting the identification. While MSI-levels for assigning metabolite identification confidence can be refined and more detailed. neither confidence thresholds nor combining different levels of experimental and biological probabilities have been thoroughly tested. Unlike proteomics, robust workflows that result in solid FDR-associated automatic structure assignments are missing in metabolomics. New methods are needed that instead focus on probability-based assessments of identification along with methods for estimating identification false discovery and that remove the subjectivity on the part of the data reporter. In this workshop, we will discuss conceptual models for assigning a probability to guantify the evidence for the presence of a compound in a sample and that are ideally generalizable and transferable across measurement platforms and sources of evidence. The role of reference libraries and their impacts in terms of size and composition will also be discussed.





#### **TUESDAY WORKSHOPS**

#### 14 Achieving Harmonized Clinical Laboratory Testing: Current Best Practices & Future Approaches Clinical Chemistry Interest Group Presiding: Candice Ulmer; Donald Chace Room 105 AB

To ensure high quality clinical laboratory testing, consistent disease diagnosis, and improved patient outcomes, the harmonization of processes for both screening and diagnostics must be achieved on a local, national, and international level. Discussions are needed on clinical laboratory best practice policies, procedures, and processes/systems to eliminate existing barriers and facilitate the comparability of laboratory information across the entire testing process. This workshop will [1] identify common QA/ QC issues in clinical laboratory testing, [2] highlight current best practices for pre-analytical, analytical, and post-analytical process, and [3] discuss considerations for new approaches to harmonize clinical laboratory testing. In addition, this workshop will provide an overview of successful quality assurance programs in clinical testing from national and international stakeholder organizations.

# WEDNESDAY WORKSHOPS

### 01 From Theory to Revolutionary Instrumentation: Nothing is More Practical than a Good Theory? Fundamentals Interest Group Presiding: Alexandre Shvartsburg; Alexander Makarov Ballroom A

We will focus on the connection between theoretical advances in ion dynamics and novel MS instrumentation, discussing the fundamental underpinnings and limitations of breakthrough MS platforms that revolutionized mass spectrometry since 2000.

Recent history of MS amply showcases the "Nothing is more practical than a good theory" dictum by US psychologist Kurt Lewin. New (often seemingly esoteric) physical concepts and developments in ion motion simulations were translated into novel MS systems of unprecedented resolving power and sensitivity providing analytical capabilities previously deemed beyond reach.

We will seek to identify the key conditions that precipitated the transition from theory (often around for decades) to the technological breakthrough. A juxtaposition to the above quote is "The great tragedy of science - the slaying of a beautiful hypothesis by an ugly fact" (Thomas Huxley). Commonly that happens to the initial model, and progress to practical implementation requires refined understanding. We will explore this yin-and-yang dynamics in several areas, tentatively:

- Ultrahigh-resolution MS: from the Kingdon trap physics to Orbitrap MS
- Ultrahigh-resolution IMS: from the traveling-wave and synchrotron IMS concepts to Cyclic IMS
- High-resolution FAIMS: leveraging the non-Blanc effects in gas mixtures
- Electron Capture Dissociation: from a peculiar FTICR feature to mass-market technology

# 02 Ambient MS and Direct to MS: Strategies for Quantitation

#### Ambient Sampling & Ionization Interest Group Presiding: G. Asher Newsome; Germán Gómez-Ríos Ballroom B

The ease and approachability of ambient ionization and direct to MS sources have made them popular methods for qualitative analysis since the mid-2000s, but the operational elements that allow

speed and minimal-to-no sample preparation are often at odds with the requirements for quantitation. At ASMS 2019, workshop attendees responded to a poll by rating "quantitative capabilities" and "reproducibility" as the top challenges in ambient ionization. Having discussed reproducibility (and lack of reproducibility) with short, virtual talks at the 2020 Reboot, this year we will host a panel of experts with hands-on experience to discuss challenges and strategies for quantitation with various sampling and ionization methods and analytes. The panel Q&A will be preceded by several 3-minute lightning talks selected from 2021 posters to share hot topics in ambient sampling and ionization. The workshop aims to encourage audience participation and presentations from new investigators, postdocs, and graduate students with a balanced perspective from inside and outside academia. The workshop will also review the new status as an interest group and solicit topics for discussion in future years.

# 03 Interpreting Imaging MS Data at 'Omics Level: Integration with Other Omics Platforms Imaging MS Interest Group Presiding: Alison Scott; Jens Soltwisch

Room 201 ABC

Progress continues to be made in interpreting imaging mass spectrometry data at the omics level and validating imaging results with other omics techniques for comprehensive spatial omics. From these investigations, several new software tools and experimental strategies have emerged to more confidently interpret metabolomics and proteomics imaging MS data in biological and pathological contexts. In this workshop, we will discuss these tools, their strengths and how to address current limitations. Preliminary topics to be addressed include:

1) Current software solutions for omics level interpretation of imaging MS data

2) Pathway analysis integration with IMS

3) How to integrate imaging interpretation software with other omics software

4) Advanced analytical methods for validation of identities in imaging MS

5) Quantitation

The workshop will entail short presentations by students, postdoctoral fellows, investigators from industry, academia, and government laboratories. Each presentation will be followed by a 5-10 minute discussion within the interest group. A goal is to



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further disseminate information on challenges and solutions for integration of imaging MS with other omics platforms for confident biological interpretation.

#### 04 Ion Mobility MS Data Analysis Tools: What's There and What Isn't Ion Mobility MS Interest Group Presiding: Ian Webb: Kelly Hines: Xuevun Zheng Room 204 ABC

The rapid development and adoption of ion mobility-mass spectrometry (IM-MS) instrumentation and methods has led to the production of data from a huge variety of experiments. The multidimensional data that is generated by IM (e.g., LC/IM/MS/ MS) is incredibly rich due to the high peak capacities of each dimension. However, the complexity of recent experiments and the resulting data have outpaced the existing capabilities for IM-MS data analysis and interpretation. The demand for these new tools is exacerbated by the unique data architectures used by each of the major IM-MS instrumentation vendors. Thus, the development of a suite of cross-platform data analysis, informatics and visualization tools for multidimensional IM-MS experiments is critical to the advancement of the field.

There have been many software tools developed by both the vendors and the users to analyze IM data. For instance, IM-MS tools that currently exist include software for IM-MS feature finding and deconvolution, targeted quantitative measurements, native MS structural analysis, and others. The workshop will provide the community with an overview of the ion mobilitymass spectrometry software tools that have been developed and their applications. This workshop will emphasize diverse topics focusing on the many types of experiments that are performed with IM-MS, including quantitative and qualitative studies ranging from metabolite and small molecule analysis to native IM-MS/ structural proteomics. We intend to provide a venue for discussion of the various capabilities and applications of the available tools and give the community an opportunity to discuss their unique applications that may not have the necessary tools available.

#### 05 The International Metaproteomics Initiative: **Communicating and Advancing Metaproteomics Research** Presiding: Pratik Jagtap; Robert Hettich; Timothy Griffin Room 102 AB

Mass spectrometry-based metaproteomics research has experienced rapid and recent growth due to its ability to help understand how microbiomes function. Leading metaproteomics researchers from multiple countries recently announced the launch of the Metaproteomics Initiative (www.metaproteomics. org). This global initiative aims to promote the dissemination of metaproteomics fundamentals, analytical and bioinformatic advancements, and applications via a collaborative communitybased network focused on microbiome research. The Initiative will maintain a central information hub where newcomers and experts can interact to communicate, share ideas and data, and accelerate experimental and bioinformatic methodologies in this field.

The workshop will introduce the Initiative along with information on how interested researchers can join, participate and contribute to the growth. The workshop will also include an update on the

Initiative's latest projects and publications. We will invite a panel of leading metaproteomics experts who will participate in a discussion that spans topics such as their motivation in joining this initiative; the current status of metaproteomics and potential challenges and opportunities in metaproteomics. The panel will also interact with the audience and address discussion points on how the initiative will help in gaining deeper insights into microbiome dynamics.

#### 06 MS Libraries for Compound Identification Presiding: Xiaoyu Yang Room 103 ABC

Panelists: Oliver Fiehn, Stephen Stein, Tim Stratton

Mass spectral (MS) libraries are widely used in almost all areas of science seeking the identification of molecules. The objective of this workshop is to provide an up-to-date forum on the latest development of MS libraries and for participants to share their related experience, suggestions, problems and concerns. The workshop will focus on the practical use and application of the MS libraries and associated software tools for compound identification. A workshop presider will first give an overview of the MS library application in human health, food, and environmental analysis. Three experts (panelists from academia, industry and government) will then describe recent developments, their insights and opinions about MS libraries, applications, and useful software tools that they utilized in their studies and projects. After a short Q&A session, the discussions will be led by the panelists and topics will include: available MS libraries, their features and limitations for LC/MS/MS and GC/MS data analysis in metabolomics, (glyco)proteomics, lipidomics, forensics, and environmental studies; library searching methods, software tools and their pros and cons; integration of libraries in other software platforms (e.g. Skyline); combining library searching with peptide sequence database searching; applying artificial intelligence (AI) in spectral prediction for compound identification. At the end of the workshop, we hope participants will learn how MS libraries can efficiently help their data analysis and what software tools can make it easier.

#### 07 Developing World Outreach

#### Developing World Outreach Interest Group Presiding: Kym Faull; Hendrik Kersten; Giles Edwards Room 104 AB

The idea is to bring together members of our society who wish to contribute to mass spectrometry related education and research in the Developing World. This goal is considered by some as an important step toward addressing issues mankind is facing, and will be facing in future. One central point is the transfer of discarded, but still running instruments to institutions in countries that could otherwise not afford them. However, there is a long way from goodwill to meaningful scientific data, paved with administrative, technical and educational hurdles. Sustainable development requires a committed network of experienced mass spectrometrists who can provide on-site installations, training, potential equipment for donation and contact persons who are prepared to share knowledge, time, and expertise. The News and Views section of the October 2019 JASMS issue broadly informed our society about the current efforts



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and needs, in particular about the work of RORO (Recycling Organization Research Opportunities), a registered charity organization operating in this field since 2006. To maintain the momentum and further develop this network we need to meet, discuss and organize things at this year's workshop. The agenda includes a report on the current status and capabilities of RORO and a broad discussion centered on bringing mass spectrometry to the Developing World. The session will be jointly organized and chaired by Kym Faull, Hendrik Kersten, Giles Edwards and Abraham Badu.

#### 08 Networking for Scientists: Celebrating Women Mass Spectrometrists Presiding: Komal Kedia; Anumita Saha; Erin Baker Room 108 AB

This year's workshop will offer participants ample opportunity to network will fellow female researchers and participate in some fun activities. Our panel will include female mass spectrometrists from various sectors as well as stages of their career. Within our panel, this year we will include a female researcher from final year of grad school/first year post-grad to provide fresh perspective on challenges and experiences of female students withing graduate school environment. Additionally, we will recruit one male PI/ manager to share advice centered around promoting gender equality within their team. The workshop will kick off with an introduction of panelists and their respective career trajectories followed by a surprise ice-breaking activity. Panelists will then share one story each in the 'PAR' format; P: problem/situation, A: action, R: result. These stories would include experiences with trying to navigate work-life balance amidst COVID pandemic amongst others. This will offer a unique viewpoint to audience in addition to providing a basis to ask more involved questions. Next, Q & A session will commence where participants can ask questions both in-live and through online portal leading to an active discussion.

#### 09 New Aspects in the Development of Multi-Attribute Method (MAM) Biotherapeutics Interest Group Presiding: Richard Rogers; Da Ren Room 109 AB

The advances of new indication and therapeutic modalities in the pharmaceutical industry drives the development of new analytical methods that provide enhanced content in a more efficient manner. In the past of decade, liquid chromatography (LC)-mass spectrometry (MS)-based Multi-Attribute Method (MAM) has successfully demonstrated its capability in replacing traditional chromatographic and electrophoretic testing methods for monitoring both product and process quality attributes (Rogers et al., AAPS J, 2017). As we enter a new decade of technology and method development, MAM's utility is expanding. Recent advances in mass spectrometry instrumentation have provided novel opportunities in reforming the original MAM. The industrywide MAM Consortium inspires method development and diversity for new MAM approaches that are fitting into different application in biopharma R&D schemes. New approaches to MAM are emerging; subunit analysis-based MAM, fully automatic sample preparation, MAM for cell and gene therapies, compact MS for MAM in QC, and new data acquiring approaches like PRM. The biotherapeutic interest group workshop offers a forum for members to share and discuss those new aspects in the development of MAM.

# 10 LC-MS for Translational DMPK and Precision Medicine DMPK Interest Group Presiding: Brian Rago; Bhagwat Prasad

#### Room 110 AB

Translation of in vitro and preclinical drug metabolism and pharmacokinetic data (DMPK) to human is important for drug development. However, differences in the abundance of drug metabolizing enzymes and transporters (DMETs) between in vitro systems and preclinical and human tissues pose an important challenge in translating these data. The protein abundance characterization of DMETs by either LC-MS targeted or global proteomics and integration of these data into physiologicallybased pharmacokinetic (PBPK) models provide a key solution to this problem.

Similarly, characterization of variability in drug disposition is important for clinical study design and precision drug treatment. Since variability in drug disposition cannot be completely described by genetics, characterization of phenotypic variability is critical.

This has fostered the development of plasma-derived exosomes as liquid biopsy and endogenous biomarkers for the prediction of drug metabolism and transport. Integration of metabolomics and proteomics data PBPK models also supports data translation for better prediction of drug disposition.

This workshop will provide an update on various non-invasive and in silico approaches for drug disposition prediction that will include application of transporter proteomics in PBPK modeling, utilizing exosomes for drug disposition prediction, and DMET proteomics in precision medicine.

#### 11 Real-time Mass Spectrometry in Proteomics and Beyond Presiding: Chris Adams; Mathieu Lavallee; Devin Schweppe Room 111 AB

Computational efficiencies, stream-lined algorithms and machine learning have had a major impact in mass spectrometry-based proteomics. Data processing can now be performed at the scale of instrument acquisition. These new capabilities give rise to realtime analysis and informed instrument acquisition based upon real-time results. This Interest Group will discuss the current state-of-the-art in real-time as applied to proteomic workflows. Additionally, we will host an open forum to discuss how users, instrument vendors and software developers can collectively contribute to realizing further advances in real-time mass spectrometry.

#### 12 Protips and Life Hacks for FTMS FTMS Interest Group Presiding: Lissa Anderson; Chad Weisbrod Room 113 ABC

Did you know that mass measurement accuracy can be significantly improved by employing calibrants that have charge distributions like those of the analytes of interest? Ever wonder



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what the difference between reduced and full profile modes was? Users of FTMS cannot all be instrumentation experts! Most have no idea what a Hanning apodization is, let alone its effect on peak shape. The goal of this year's FTMS workshop will be to outline important considerations for FTMS and distill relevant information in the simplest way possible for end users. Speakers will be recruited from academia and industry to provide expert advice tailored to those of us who don't know how to use SIMION. Check out the FTMS interest group website for updates. Presentations and workshop minutes will be made available.

#### 13 Trans-Proteomic Pipeline: Recent Advances and Future Directions

#### Presiding: Michael Hoopmann; David Shteynberg Room 114

The workshop will begin with a brief overview of the Trans-Proteomic Pipeline (TPP) and its newest features and capabilities. We will then focus on four 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 their challenges in proteomic data analysis and help drive directions in software approaches through needs of the community. The topics for discussion will be focused on the new functionalities in the upcoming TPP version 6.0.0 release, including but not limited to:

- Quantitation techniques employing isobarically labeled samples acquired on timsTOF
- Quantitation techniques from timsTOF DIA datasets
- Predicting peptide ion mobility values with machine learning
- Evaluating digestion efficiency in datasets

Each topic will be introduced with a brief summary of features and ideas. Then feedback and discussion by the workshop participants will be promoted.

#### 14 Utilization of Mass Spectrometry in Cannabis & Hemp Analysis Presiding: Asra Gilani, Eberhardt Kuhn Room 105 AB

The global legalization of cannabis and hemp-derived medicine and consumer products has paved the way for advances in cannabis science- from the accurate detection of active cannabinoids and harmful, trace contaminants to more informative strain typing, advanced breeding programs and clinical research.

Mass spectrometry is playing an increasingly important role in product quality and compliance safety testing. This testing requires accurate identification and quantification of the analytes of interest in often challenging matrices to low detection requirements (ppb). This session will review applications of MS in regulatory environments, quality control testing labs as well as emerging academic, clinical and industrial areas, including advanced agricultural, nutritional and bioscience programs. Join us as we review and discuss current and future applications of mass spectrometry in advancing cannabis/hemp science.

#### Goals:

- Foster discussions regarding the applications of mass spectrometry to cannabis and hemp markets.
- Deliver key opinion leader panel discussions on regulatory environments, QC testing and other markets as well as future directions.
- Encourage expanded use of mass spectrometry in cannabis/hemp applications by sharing information and discussing emerging growth areas.

#### Presentations & Panelists:

- "The Role of Mass Spectrometry in the Cannabis Industry", Jack Henion, Co-Founder and CSO (Retired), Advion, Ithaca, NY, and Emeritus Professor of Analytical Toxicology, New York State College of Veterinary Medicine, Cornell University
- "Regulatory Science Applications of Mass Spectrometry in Cannabis and Hemp Testing", Volker Bornemann, President and CEO, Avazyme
- Utilizing Mass Spectrometry to Identify Pharmacologically Active Compounds in Hemp", Richard van Breemen – Principal Investigator, Linus Pauling Institute, Professor of Medicinal Chemistry, Department of Pharmaceutical Sciences, College of Pharmacy, Oregon State University

# **15 Metabolomic Applications in Human Health and Environmental Sciences** *Metabolomics Interest Group* Presiding: Maryam Goudarzi; Thomas Horvath

#### Room 107 B

Advances in analytical workflows, instrumentation, and improved data analytics have led to significant growth in the field of metabolomics over the last decade. Direct application of metabolomic techniques in the biomedical and environmental research settings are the topic of this workshop. We will hear from Dr. Douglas Walker (exposomics; Mount Sinai Medical Center) and Dr. Melinda Engevik (microbiome and mammalian gut-brain axis; Medical University of South Carolina) on how they apply metabolomic techniques to their research. The main presentations will be followed by four 5 min lightening talks given by early-career scientists under the same suggested theme. There will be a panel discussion where the speakers will engage with the participants in a free-discussion format. During the workshop the attendees will be asked to vote to select the best presentation from the four lightening talks via a live polling mechanism. The winner will be announced at the end of the workshop. We believe that this workshop will provide an excellent opportunity for early-career investigators to gain access to the broad experience base present in the Metabolomics Interest Group.

> Consult online planner or mobile app for detailed program. Also includes content for in-person and remote posters.





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