AMERICAN SOCIETY OF
MASS SPECTROMETRY

70th Conference on Mass Spectrometry and Allied Topics

Minneapolis 2022

JUNE 5-9
Minneapolis, Minnesota

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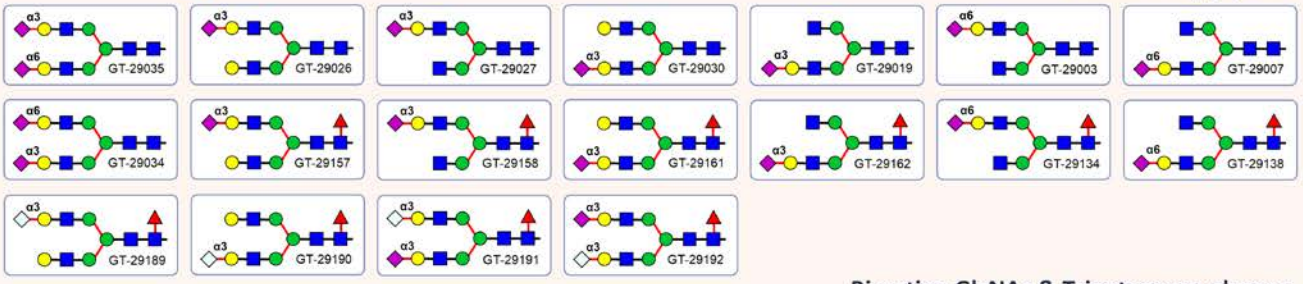

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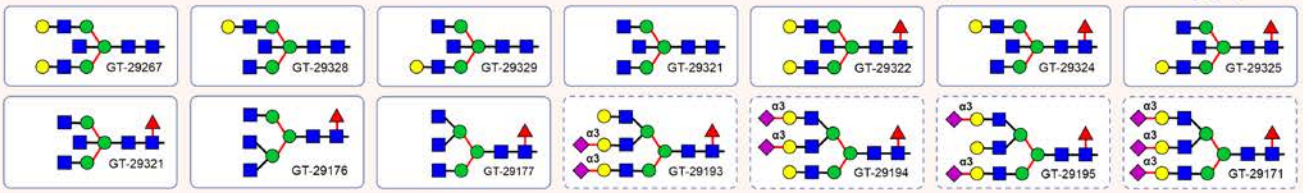

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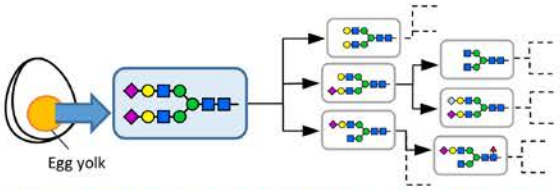

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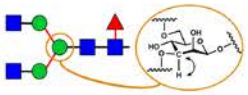
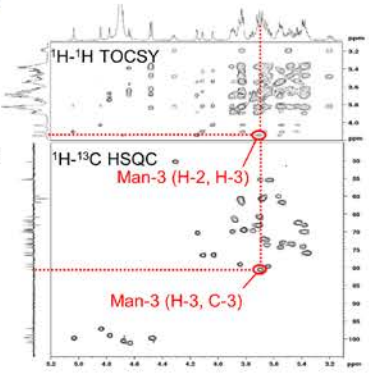


^{1}H-^{13}C correlation signal of 3-position of Man-3



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Welcome to the 70th ASMS Conference on Mass Spectrometry and Allied Topics. Conference program activities and exhibit booths are in the Minneapolis Convention Center. Corporate Hospitality Suites are at the Hilton Minneapolis.

SPONSORS

ASMS gratefully acknowledges the support of the following.

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TABLE OF CONTENTS

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

Attention
Undergraduate Students and First Time (at ASMS) Graduate Students
4:00 - 4:45 pm, Sunday, Hall A
Plan Your Strategy: What to See and Do at ASMS

Tutorial Session I, Hall A
5:00 – 5:45 pm
Mass Spectrometry in Biopharma: From Small Molecules to Multi-Specific Antibodies and Beyond

Iain D. G. Campuzano
Amgen Research

5:45 – 6:30 pm
Machine Learning in Mass Spectrometry

Randy Julian
Indigo BioAutomation

Tutorial Session II, Rm L100
5:00 – 5:45 pm
Radical Chemistry for Biomolecular Identification: From Fundamentals to Applications

Ryan R. Julian
University of California, Riverside

5:45 – 6:30 pm
Mass Spectrometry in Natural Product Research

Laura Sanchez
University of California, Santa Cruz

Sunday Conference Opening 6:45 - 7:45 pm, Hall A

Opening Remarks

Julia Laskin
Purdue University
ASMS Vice President for Programs

Of Stem Cells, Niches and Networks

Judith Kimble
University of Wisconsin-Madison

Sunday Welcome Reception 7:45 - 9:00 pm, Halls BC
Conference name badge is required.

Monday Award Lecture 4:45 - 5:30 PM, Hall A

John B. Fenn Award for a Distinguished Contribution in Mass Spectrometry

Evan R. Williams
University of California, Berkeley

Tuesday Award Lecture 4:45 - 5:30 PM, Hall A

Biemann Medal

Erin Baker
North Carolina State University

Wednesday ASMS Meeting 4:45 - 5:30 PM, Hall A

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

Thursday Plenary Session 4:45 - 5:30 PM, Hall A

Homo naledi and the Chamber of Secrets

Jeremy DeSilva
Dartmouth College

Thursday Closing Event 6:30 - 10:30 PM, Hall D
Advance Purchase Ticket Required
Ticket Sales Close 12pm noon, Monday June 6

Buy your ticket online via Registration portal. If you purchase after printing your name badge, you will need to re-print your badge.

Join us for a funky, music filled evening featuring the official Prince tribute band PurpleXperience. Light supper served before the concert. Get ready to DANCE! Location is Hall D of the convention center.

Consult online planner or mobile app for detailed program.

Oral Sessions are 8:30 - 10:30 am and 2:30 - 4:30 pm Monday through Thursday.

Session A (MOA, TOA, WOA, ThOA)..... Hall A
Session B (MOB, TOB, WOB, ThOB) .....Room L100
Session C (MOC, TOC, WOC, ThOC) ..... Ballroom A
Session D (MOD, TOD, WOD, ThOD) .....Ballroom B
Session E (MOE, TOE, WOE, ThOE) ..... Auditorium
Session F (MOF, TOF, WOF, ThOF).....Room 101
Session G (MOG, TOG, WOG, ThOG) .....Room 102
Session H (MOH, TOH, WOH, ThOH) .....Room 103

Oral Presentations are projected from ASMS computers running Microsoft Office. Speakers are required to use the ASMS computers for their presentations.

Speakers must load presentations at least one day prior to their talks. The speaker ready room is Room M101 ABC. The room is open with a technician according to this schedule:

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

Posters and Exhibit Booths, Halls BC. 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

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

Poster Sessions are 10:30 am - 2:30 pm, Monday through Thursday.

Poster Authors must be present at posters on scheduled days at these times. 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.

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

Exhibitors must staff exhibit booths as follows:

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

Workshops are 5:45 - 7:00 pm on Monday, Tuesday, and Wednesday. Light refreshments are provided.

Special Program for Undergraduate Students

- **Sunday, 7:30 - 9:00 pm, Poster competition**, Poster/Exhibit Hall (pre-registration required)
- **Monday, 11:30 am - 1:00 pm, Meet the Experts.** Lunch tables are reserved for undergraduate students in the Poster/Exhibit Hall. Voucher for lunch at concessions will be provided at tables. Arrive promptly at 11:30 am to obtain your voucher.

Free WiFi Access is available throughout the convention center, use the ‘ASMS’ network with password: asms2022 (case-sensitive).

Career Center is located in Room 208AB. The Career Center is open to all conference attendees. Applicants and employers must enter resumes and employment opportunities online. There are computers in the center for searching the database of candidates and positions. Interview rooms are available nearby and should be reserved one-day in advance.

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

Gender Neutral Restrooms throughout the convention center.

Mother’s Lounge is in Room 201 A. This room is intended for use by nursing mothers.

Closing Event, $40 on Thursday evening requires an **advance purchase ticket**. Ticket sales CLOSE on Monday June 6, 12pm noon. Buy your ticket online via Registration portal. If you purchase after printing your name badge, you will need to re-print your badge.

Join us for a funky, music filled evening featuring the official Prince tribute band PurpleXperience. Light supper served before the concert. Get ready to DANCE! Location is Hall D of the convention center.

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.

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

All **Health & Safety Plan** protocols in effect for a specific conference must be followed by all conference attendees and their companions.

Name badge is required for all conference sessions, short courses, and conference-related events (hospitality suites, closing event.)

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

No photography or recording is allowed in oral sessions or in the poster hall.

Publicity Release. By attending or participating in an ASMS event, attendees agree to allow their names, likenesses, and images, in audio, photographic or video format recorded for the event and onsite, to be used by ASMS for educational, promotional, or marketing of ASMS events or activities.

Material presented or displayed at the ASMS Conference, including but not limited to orals, posters, workshops, exhibit booths and hospitality suites, is the intellectual property of the presenter and may not be recorded, photographed, quoted, disseminated or transmitted by summary in any form without express written authority of the author. If you wish to cite an abstract presented at the annual conference, please use the citation guidelines for conference proceedings found at asms.org.

The placement of advertising in the meeting area is prohibited. There are poster boards and tables in the Poster/Exhibit Hall for approved announcements. Ask at Registration desk to have your announcement approved.

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

No organized activities (even off-site) other than those approved by ASMS are allowed during the conference week (5:00 pm on Sunday through 6:00 pm on Thursday).

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

Parents. Conferences during the pandemic will mean that **all** persons in the conference space must follow any prescribed Health & Safety Plan protocols in effect for the event. This includes accompanying persons and children age 5 and older. The following applies to children under age 5 and infants:

- Children age 2 and older must follow any masking guidelines in effect
- Children under age 5 are not subject to any proof of vaccination or negative test result

In general, ASMS provides the following advice for parents considering bringing child(ren) or infant(s): Planned conference sessions and hospitality suites may **not** be appropriate for children. Please respect the interests of your colleagues to attend activities without disruption and without concern for the safety of children. Strollers, child backpack carriers or similar devices are permitted in the poster hall, and with careful supervision by parents. Strollers are prohibited in the hospitality suites.

THURSDAY CLOSING EVENT

Dinner & Concert by PurpleXperience

ADVANCE PURCHASE TICKET REQUIRED

TICKET SALES CLOSE 12PM NOON, MONDAY JUNE 6

Buy your ticket online via Registration portal. If you purchase after printing your name badge, you will need to re-print your badge.

Join us for a funky, music filled evening featuring the official Prince tribute band PurpleXperience. Light supper served before the concert. Get ready to DANCE!

Thursday, June 9, 6:30-10:30 pm. Advance purchase ticket required.

NETWORKING OPPORTUNITIES

Special Gap Hour Receptions

Monday & Tuesday 7:00-8:00 PM

Monday, 7pm / Room 101

FeMS Reception

Sponsored by Agilent

Immediately following Celebrating Women Mass Spectrometrists evening workshop.

Come network with the FeMS community!

Tuesday, 7pm / Ballroom A

Diversity & Inclusion Reception

Sponsored by MOBILion

Immediately following evening workshop organized by the ASMS D&I Committee.

Interested in issues of diversity, equity, and inclusion? Join us to network and create community!

LOOK HISTORY POSTERS

Main foyer near entrance to Posters-Exhibits.

Funding Agency Office Hours

Inside Posters-Exhibits Hall Monday-Thursday 10:30 am - 2:30 pm. Meet with representatives from various funding agencies. Appointment sign-up sheets will be posted on 'office' entry sign (along main entry inside posters-exhibits area).

Attendees are encouraged to take advantage of this valuable resource while at the conference.

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CONGRATULATIONS
to these members who are elected to serve on the ASMS Board. Their terms begin July 1, 2022

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Biotherapeutics	Da Ren Richard Rogers
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Flavor, Fragrance and Foodstuff	Joe Binkley Travis Falconer
Forensics & Homeland Security	Brittany Casey Ruth Smith Waddell
FTMS	David Butcher Chad Weisbrod
Fundamentals	Alexander Makarov Alexandre Shvartsburg
H/D Exchange, Covalent Labeling & Cross Linking	Fabio Gozzo Corie Ralston
Imaging MS	Angus Grey Alison Scott
Ion Mobility MS	Kelly Hines Xueyun Zheng
Ion Trap MS	Theresa Evans-Nguyen Dalton Snyder
LC/MS Related Topics	James Dodds Jack Ryan
Lipids & Lipodomics	Michael Holčapek Harold Köfeler
Metabolomics	Maryam Goudarzi Thomas Horvath Tytus Mak
Native MS	Ashley Bell Justin Benesch Liz Hecht
Pharmaceuticals	Angela Calderon Kiran Iyer
Photoionization MS	Luke Hanley Matthias Lorenz Christopher Rueger
Polymeric Materials	Thierry Fouquet Jessica Hoskins
Regulated Bioanalysis	Dian Su Jian Wang
Top-Down Proteomics	Caroline DeHart Mowei Zhou
Undergraduate Research in MS	Brandie Ehrmann Kate Stumpo
Young Mass Spectrometrists	Christopher Pulliam Laura Sanchez

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History	P. Jane Gale, Chair Asher Newsome Ron Hites Magnus Palmblad Adrienne Tymiak Michael Grayson, *ex-officio*
Nominating	Jennifer Brodbelt, Chair Tarun Anumol Lan Huang Christina Jones Touradji Solouki
Publications	Stephen Valentine, Chair Richard Y. Huang Vanessa Phelan Si Wu Mowei Zhou Joseph Loo, *ex officio*
Sanibel Conference	Lissa Anderson, Chair Xiuxia Du Richard Rogers Ljiljana Pasa-Tolic (ASMS Board Rep.)

JOHN B. FENN AWARD FOR A DISTINGUISHED CONTRIBUTION IN MASS SPECTROMETRY

2022 Recipient: Evan R. Williams
Award Lecture: 4:45 PM, Monday, Hall A

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. 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.

Evan R. Williams is the recipient of the 2022 ASMS John B. Fenn Award for a Distinguished Contribution in Mass Spectrometry for the development of ion chemistry in aqueous nanodrops: fundamentals and applications. Dr. Williams has made pioneering contributions that have improved our fundamental understanding of ion chemistry in aqueous nanodrops both inside and outside the mass spectrometer. His work has had tremendous impact and represents a cohesive and successful sustained effort to understand the chemistry occurring in aqueous solution during the transition in the electrospray process from bulk solution to individual ions or solvated ions.

He has taken advantage of nanodrop chemistry to: 1) manipulate ion charging and desalting ions during the electrospray ionization process, 2) develop rapid mixing in electrospray droplets to investigate ultrafast chemistry (<1 to 100 microseconds) to track peptides and fast-folding proteins in the act of folding, 3) investigate how the organization of water around ions can pattern the hydrogen bonding network of water to long distance, and how water can affect the structure of ions, and 4) develop thermochemical methods, including blackbody infrared radiative dissociation and ion nanocalorimetry, to probe the thermochemistry of processes, such as electrochemical reductions in mass selected aqueous nanodrops.

This collective theme has influenced not just the field of mass spectrometry and ion chemistry but has also improved our understanding about the role of water on ion chemistry in solution, an outcome which impacts many areas ranging from biomolecule structure and folding to atmospheric aerosol chemistry.

Dr. Williams is a Distinguished Professor of Chemistry and Biophysics, University of California, Berkeley.

BIEMANN MEDAL

2022 Recipient: Erin Baker
Award Lecture: 4:45 PM, Tuesday, Hall A

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

Erin Baker is the recipient of the 2022 ASMS Biemann Medal for her significant contributions in the development and application of IMS-MS technologies. The impact of her work has been amplified due to her notable and unique ability to form a bridge between the new IMS-MS technology development and the diverse applications the technology enables. Examples of innovative scientific contributions include: (1) development of new IMS techniques and methods and significant contributions to the improvement of drift tube IMS (DTIMS) platforms; (2) coupling of this improved IMS-MS platform with solid-phase extraction and LC separations to enable high-throughput IMS measurements with enhanced sensitivity for metabolomics, lipidomics, proteomics and exposomics applications; (3) creation of one of the first collision cross section (CCS) databases for more than 500 metabolites and xenobiotics to enable large-scale metabolomics and exposomic studies by IMS technology; and (4) development of a cheminformatic toolbox called Structural-based Connectivity and Omic Phenotype Evaluations (SCOPE), to enable the assessment and visualization of lipidomic associations in environmental and clinical studies.

In addition, Dr. Baker has contributed to the mass spectrometry community through her key role in the establishment of the new group “Females in Mass Spectrometry (FeMS)” whose initial activities coincided with the onset of the coronavirus pandemic. During this unusual situation that has isolated individuals from their communities, FeMS has built a worldwide network (also including males, transgender, and nonbinary participants) that provides frequent virtual opportunities for education, collaboration, and mentorship.

Dr. Baker is Associate Professor of Chemistry, North Carolina State University.

AL YERGY MS SCIENTIST AWARDS
2022 Recipients
Award Presentations: ASMS Meeting, 4:45 PM, Monday, Hall A

The Al Yergey MS Scientist Awards are sponsored by ASMS to recognize dedication and significant contributions to mass spectrometry-based science by "unsung heroes." The awards are named in memory of Al Yergey a well-respected scientist who was known as a dedicated mentor. Each award is conferred at the ASMS Annual Conference with $1,000 cash award and a recognition memento.

Gordon A. Anderson is recognized for his immense, impactful, and sustained contributions to mass spectrometry. His technical contributions, strength of character, and mentoring of junior scientists exemplify the spirit of the Al Yergey Award. Gordon is now the chief engineer of a family run enterprise (GAA Custom Electronics) that broadly serves the MS community with a range of innovative and highly functional MS-specific electronic solutions.

Michael A. Grayson has championed the cause of history for the Society as archivist, historian, oral history interviewer, and the ASMS representative to the Heritage Council of the Science History Institute. His dedication to preserving the history of significant individuals and events has resulted in the rich resources available through asms.org. Now retired, Michael continues to actively contribute to the many projects of the ASMS History Committee.

Martha M. Vestling has contributed to MS-based research, extensive service to the MS community, and dedication to education and training of students and users from diverse scientific backgrounds for five decades. As the Director of the Mass Spectrometry Laboratory at University of Wisconsin-Madison, she has developed a "go-to" facility for researchers on campus and many other biomedical science departments and units.

RON HITES AWARD OUTSTANDING RESEARCH PUBLICATION IN *JASMS*
Award Presentation: ASMS Meeting, 4:45 PM, Wednesday, Hall A

The Ron Hites Award recognizes an outstanding publication of original research published in JASMS. 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.

Elyssia Gallagher, Assistant Professor, Baylor University, is recipient of the 2022 Hites Award along with co-authors O. Tara Liyanage, Ana V. Quintero, Jacob B. Hatvany for their paper "Distinguishing Carbohydrate Isomers with Rapid Hydrogen/ Deuterium Exchange-Mass Spectrometry;" *J. Am. Soc. Mass Spectrom.* (2021) **32**, 152-156

2022 RESEARCH AWARDS
Award Presentations: ASMS Meeting, 4:45 PM, Wednesday, Hall A

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

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University of Georgia

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Gloria Sheynkman
University of Virginia

Sponsored by Waters THE SCIENCE OF WHAT'S POSSIBLE.™

Thanh D. Do
University of Tennessee-Knoxville

Research At Primarily Undergraduate Institution (PUI) Award
Award Presentation: ASMS Meeting, 4:45 PM, Wednesday, Hall A

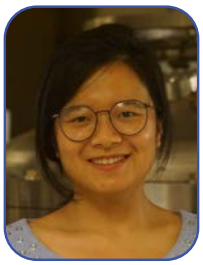
Sponsored by Agilent

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.

Mac Gilliland
Furman University

2022 POSTDOCTORAL CAREER DEVELOPMENT AWARDS
Award Presentations: ASMS Meeting, 4:45 PM, Wednesday, Hall A

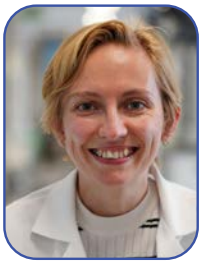
Postdoctoral Career Development Awards in the amount of $5,000 promote professional career development of postdoctoral fellows in the field of mass spectrometry.



Yangjie Li
Stanford University

Xin Ma
Georgia Institute of Technology

Melissa Pergande
University of Wisconsin-Madison



Stephanie Rankin-Turner
Johns Hopkins University

Hua Zhang
University of Wisconsin-Madison

2022 GRADUATE STUDENT TRAVEL AWARDS
Award Presentations: ASMS Meeting, 4:45 pm, Wednesday, Hall A

Hongxia Bai
North Carolina State University

Alexandria Battison
University of Connecticut

Hsi-Chun Chao
Purdue University

Janine Fu
University of California, Los Angeles

Michael Gilbert
University of Pennsylvania

Jian Guo
University of British Columbia

Hang Hu
Purdue University

Jacob Jordan
University of California, Berkeley

Kaylie Kirkwood
North Carolina State University

Zachary Kirsch
University of Massachusetts, Amherst

Gordon Luu
University of California, Santa Cruz

Jake Melby
University of Wisconsin-Madison

Hannah Miles
University of Wisconsin-Madison

Alice Passoni
Istituto di Ricerche Farmacologiche Mario Negri IRCCS

Amber Rolland
University of Oregon

Jonathan Specker
University of Florida

Diana Velosa
Florida Institute of Technology

Shunyang Wang
University of California, Davis

Tian Xu
Michigan State University

Dong Zhang
Texas Tech University

2022 UNDERGRADUATE STUDENT TRAVEL AWARDS
Award Presentations: ASMS Meeting, 4:45 pm, Wednesday, Hall A

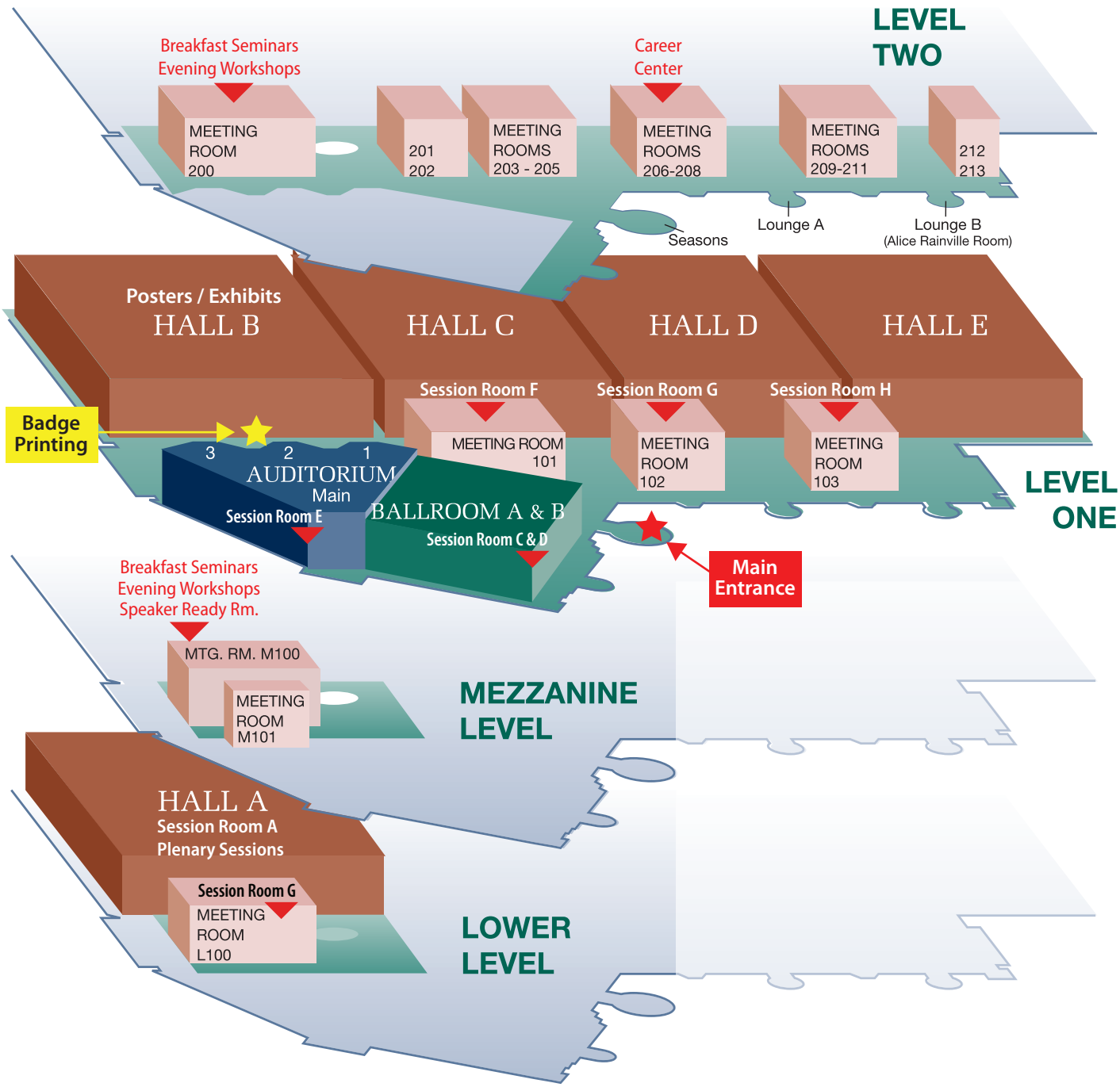
Mustafa Ahmed
George Washington University

Nickolas Fisher
University of Texas, Austin

Keely Fuller
Stanford University

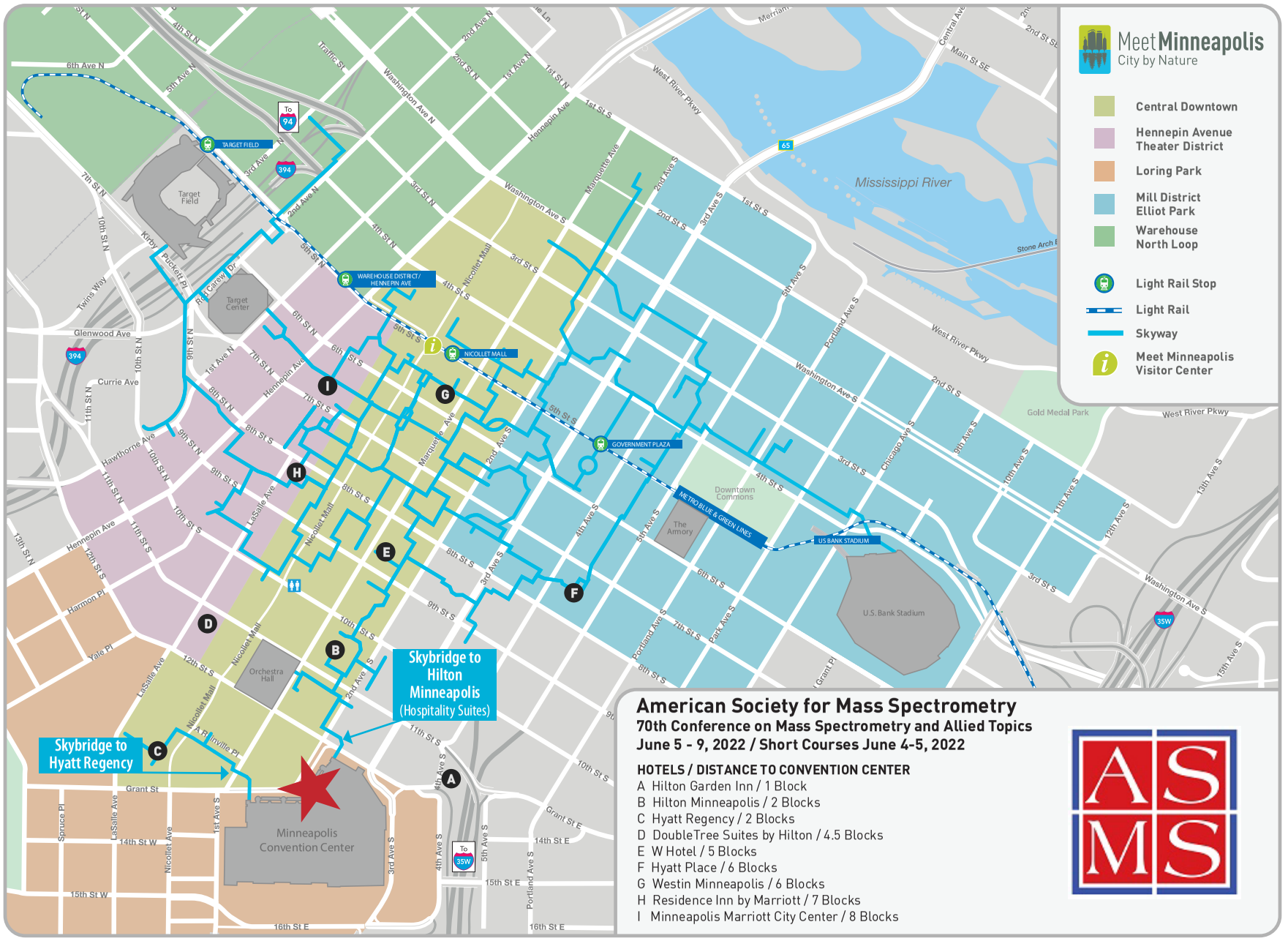
Peter McPike
University of Akron

Hsu-Ching Yen
University of Wisconsin-Madison


LEVEL TWO
Breakfast Seminars
Evening Workshops
MEETING ROOM 200
201
202
MEETING ROOMS 203 - 205
Career Center
MEETING ROOMS 206-208
MEETING ROOMS 209-211
212
213
Seasons
Lounge A
Lounge B
(Alice Rainville Room)
Posters / Exhibits
HALL B
HALL C
HALL D
HALL E
Session Room F
Session Room G
Session Room H
Badge Printing
3
2
1
AUDITORIUM
Main
Session Room E
MEETING ROOM 101
MEETING ROOM 102
MEETING ROOM 103
BALLROOM A & B
Session Room C & D
LEVEL ONE
Main Entrance
Breakfast Seminars
Evening Workshops
Speaker Ready Rm.
MTG. RM. M100
MEETING ROOM M101
MEZZANINE LEVEL
HALL A
Session Room A
Plenary Sessions
Session Room G
MEETING ROOM L100
LOWER LEVEL

MINNEAPOLIS CONVENTION CENTER - HALLS B & C

AMERICAN SOCIETY FOR MASS SPECTROMETRY HOTELS / DISTANCE TO CONVENTION CENTER



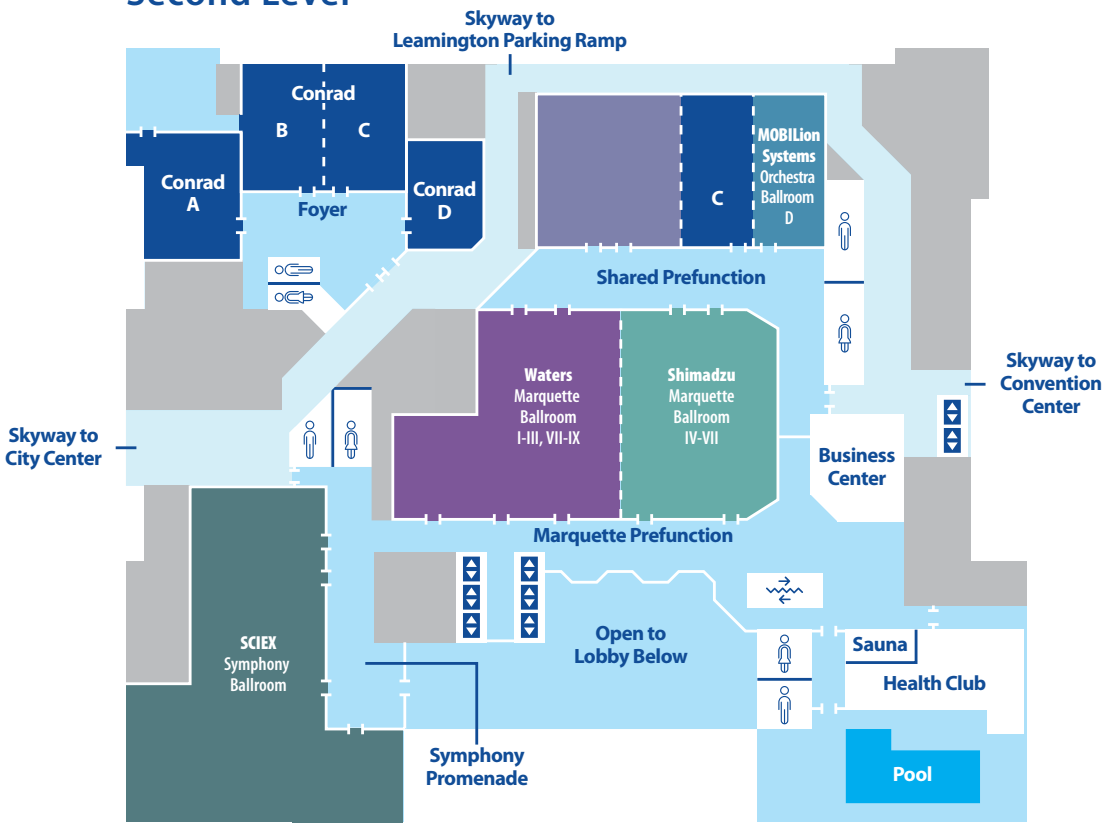
American Society for Mass Spectrometry

70th Conference on Mass Spectrometry and Allied Topics
June 5 - 9, 2022 / Short Courses June 4-5, 2022

HOTELS / DISTANCE TO CONVENTION CENTER

A Hilton Garden Inn / 1 Block
B Hilton Minneapolis / 2 Blocks
C Hyatt Regency / 2 Blocks
D DoubleTree Suites by Hilton / 4.5 Blocks
E W Hotel / 5 Blocks
F Hyatt Place / 6 Blocks
G Westin Minneapolis / 6 Blocks
H Residence Inn by Marriott / 7 Blocks
I Minneapolis Marriott City Center / 8 Blocks

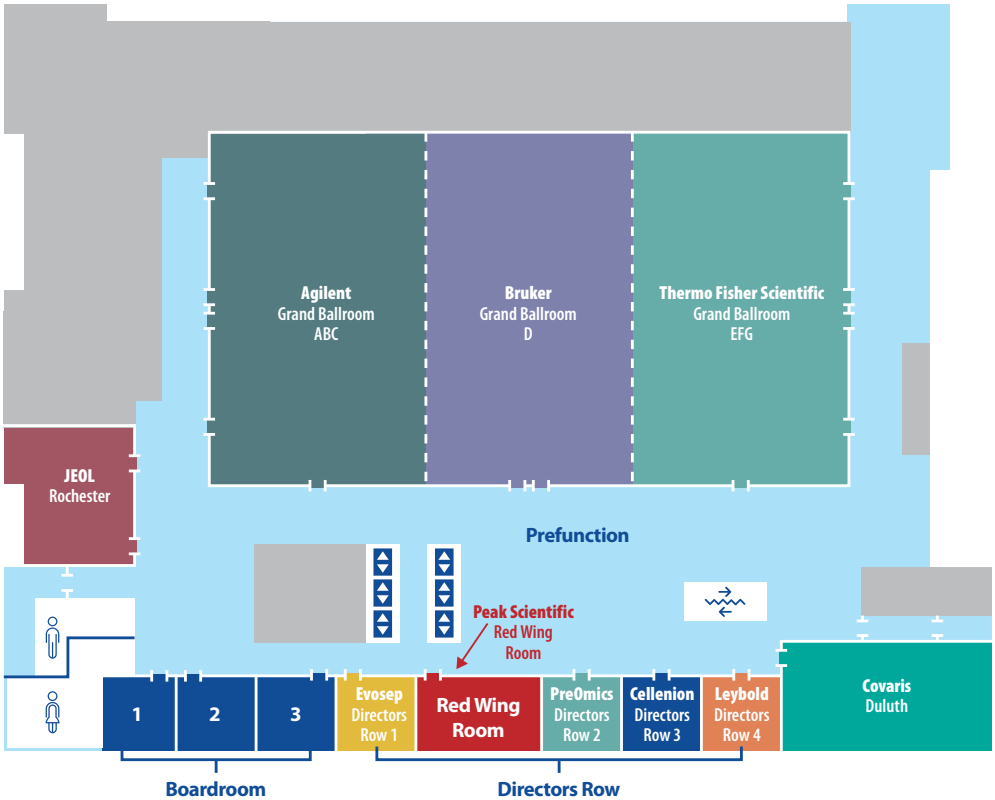
Second Level



Third Level

FLOOR MAP KEY

- Meeting/Conference Rooms
- Amenities
- Public Space
- Private
- Outdoor Space
- Stairs and Escalators
- Elevators



MEDIA EVENTS (PRESS CONFERENCES) AT HILTON MINNEAPOLIS

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

MONDAY, JUNE 6		
Time	**Company**	**Hilton Minneapolis**
9:30 - 10:30 am	Shimadzu Scientific Instruments	Marquette Ballroom IV-VII
11:00 am - 12:00 pm	SCIEX	Symphony Ballroom
1:30 - 2:30 pm	Agilent	Grand Ballroom ABC
3:00 – 4:00 pm	Thermo Fisher Scientific	Grand Ballroom EFG
4:30 - 5:30 pm	Bruker Daltonics	Grand Ballroom D
TUESDAY, JUNE 7		
Time	**Company**	**Hilton Minneapolis**
9:00 – 10:00 am	MOBILion Systems	Orchestra Ballroom D

BREAKFAST SEMINARS AT CONVENTION CENTER & HILTON MINNEAPOLIS

Breakfast Seminars are hosted by Corporate Members at the Minneapolis Convention Center and the Hilton Minneapolis. Pre-registration (RSVP) is recommended. Please look for Breakfast Seminars page on www.asms.org and in the online planner / mobile app to find online registration links for these events.

MONDAY, JUNE 6			
Minneapolis Convention Center *All breakfasts begin at 7:00 AM*		**Hilton Minneapolis** *All breakfasts begin at 7:00 AM*	
Biognosys	Room 200BC	Agilent	Grand Ballroom ABC
Bruker	Room 200DE	MOBILion Systems	Orchestra Ballroom D
Covaris	Room 200A	Thermo Fisher Scientific	Grand Ballroom EFG
Evosep	Room 200J	Waters	Marquette Ballroom I-IX
Matrix Science	Room M100BC		
SCIEX	Room 200FG		
Shimadzu	Room 200HI		
Waters	Room M100A		
TUESDAY, JUNE 7			
Minneapolis Convention Center *All breakfasts begin at 7:00 AM*		**Hilton Minneapolis** *All breakfasts begin at 7:00 AM*	
Bruker	Room 200 DE	Agilent	Grand Ballroom ABC
MassTech	Room 200A	Thermo Fisher Scientific	Grand Ballroom EFG
MOBILion Systems	Room 200BC	Waters	Marquette Ballrom I-IX
Newomics	Room 200J		
SCIEX	Room 200FG		
Shimadzu	Room 200HI		
Waters	Room M100A		
WEDNESDAY, JUNE 8			
Minneapolis Convention Center *All breakfasts begin at 7:00 AM*		**Hilton Minneapolis** *All breakfasts begin at 7:00 AM*	
Biognosys	Room 200BC	Agilent	Grand Ballroom ABC
Bruker	Room 200DE	Thermo Fisher Scientific	Grand Ballroom EFG
Phenomenex	Room 200A	Waters	Marquette Ballroom I-IX
SCIEX	Room 200FG		
Shimadzu	Room 200HI		
THURSDAY, JUNE 9			
Minneapolis Convention Center *All breakfasts begin at 7:00 AM*			
SCIEX	Room 200FG		
Shimadzu	Room 200A		
Thermo Fisher Scientific	Room 200HI & Room 200J		

Corporate Member	Exhibit Booth No. Corporate Poster Publisher Table	Hospitality Suite at Hilton Minneapolis	Breakfast Seminar at Convention Center or Hilton Minneapolis
908 Devices	409		
ACD/Labs	518		
ACS Publications	318		
Advanced Materials Technology	219		
Advion Interchim Scientific	419		
Affinisep USA	519		
AffiPro	514		
Agilent Technologies	401	Grand Ballroom ABC	
Alliance Pharma	202		
AmberGen	221		
AMETEK Powervar	818		
Analytical Sales and Services, Inc.	420		
ANCORP	719		
Antec Scientific	312		
Ardara Technologies	825		
Aspect Analytics	324		
Avanti Polar Lipids, Inc.	207		
BaySpec, Inc.	520		
BGI Americas Corporation	403		
Biocrates Life Sciences AG	618		
Biognosys	306		Breakfast Seminar(s), see pg 16
Bioinformatics Solutions Inc.	313		
Biotage	715		
Biotech Support Group	706		
Breath Explor	226		
Bruker Daltonics	407	Grand Ballroom D	Breakfast Seminar(s), see pg 16
Cambridge Isotope Laboratories, Inc.	201		
Cayman Chemical Company	308		
CDS Analytical, LLC	708		
Cellenion	713	Directors Row 3	
Cerno Bioscience	527		
CMP Scientific Corp	608		
CoAnn Technologies	421		
CovalX	625		
Covaris	412	Duluth	Breakfast Seminar(s), see pg 16
CTC Analytics AG	709		
Edwards Vacuum	724		
El-Mul Technologies	809		
Emerald Scientific	624		
e-MSion, Inc.	714		
ESI Source Solutions	327		
Evosep	418	Directors Row 1	Breakfast Seminar(s), see pg 16
Fasmatech	826		
F-DGSi	827		
Fossil Ion Technology	214		
Frontage Laboratories	820		
Genedata	426		
GenNext Technologies, Inc.	315		
Genovis Inc	424		
GenTech Scientific, Inc.	220		
GERSTEL, Inc.	614		
GlycoPath	425		

Corporate Member	Exhibit Booth No. Corporate Poster Publisher Table	Hospitality Suite at Hilton Minneapolis	Breakfast Seminar at Convention Center or Hilton Minneapolis
Hamilton Company	209		
HTA srl	325		
HTX Technologies, LLC	525		
HVM Technology, Inc.	224		
IMCS	203		
IMI Adaptas	718		
Immuto Scientific	427		
INFICON	612		
Inotiv, Inc.			
International Ceramic Engineering	626		
International Equipment Trading Ltd	303		
Ion Opticks Pty Ltd	326		
IonBench	215		
IonDX	726		
Ionoptika Ltd.	524		
Ionsense Inc.	509		
IROA Technologies LLC	700		
JEOL USA, Inc.	414	Rochester	
Lab Tech Support	506		
Larodan	821		
LCGC/Spectroscopy	720		
Lead Molecular Design	609		
LECO Corporation	408		
Leybold USA	200	Directors Row 4	
Linden CMS GmbH	Corporate Poster		
LNI Swissgas	803		
MAC-MOD Analytical	602		
Mass Dynamics	727		
MassTech Inc.	603		Breakfast Seminar(s), see pg 16
Matrix Science	415		Breakfast Seminar(s), see pg 16
Mestrelab Research	213		
MetaSci Inc.	218		
MilliporeSigma	815		
MOBILion Systems, Inc.	502	Orchestra Ballroom D	Breakfast Seminar(s), see pg 16
Moeller Medical GmbH	613		
MRM Proteomics	707		
MSAID GmbH	526		
MSTM, LLC	606		
Nest Group, Inc., The	Corporate Poster		
New Objective			
Newomics Inc.	507		Breakfast Seminar(s), see pg 16
NIST	413		
Omics Informatics	721		
Optimize Technologies	302		
Parker Hannifin	813		
Peak Scientific	615	Red Wing Room	
Pfeiffer Vacuum	500		
Phenomenex	801		Breakfast Seminar(s), see pg 16
Phoenix S&T, Inc.	309		
Photonis	513		
Phytronix Technologies	508		
Plasmion	725		

Corporate Member	Exhibit Booth No. Corporate Poster Publisher Table	Hospitality Suite at Hilton Minneapolis	Breakfast Seminar at Convention Center or Hilton Minneapolis
Polymer Factory	Corporate Poster		
PreOmics GmbH	319	Directors Row 2 (Mon, Tues)	
Promega Corporation	208		
PromoChrom	807		
Protein Metrics Inc.	701		
Proteoform Scientific	512		
Proteome Software Inc.	503		
ProtiFi, LLC	800		
QPS, LLC			
Quantum Analytics	814		
Rapid Novor Inc.	301		
Refeyn Inc.	227		
Regis Technologies	515		
Restek Corporation	212		
ReSyn Biosciences	808		
Sapphire Bioservices LLC	802		
SCIEX	501	Symphony Ballroom	Breakfast Seminar(s), see pg 16
Seer	703		
SepSolve Analytical Ltd.	627		
SeqGen	819		
Shanghai Gene Era Bio-Science	320		
Shimadzu Scientific Instruments, Inc.	406	Marquette Ballroom IV-VII	Breakfast Seminar(s), see pg 16
Shodex - Showa Denko America	206		
Sierra Analytics	521		
Silantes GmbH	812		
Sound Analytics	806		
Spark Holland B. V.	619		
Spectroswiss	601		
Spellman High Voltage	307		
SunChrom GmbH	603		
Syft Technologies	824		
Teledyne SP Devices	620		
The Analytical Scientist	Publisher Table		
The Metabolomics Innovation Centre	621		
Thermo Fisher Scientific	400	Grand Ballroom EFG	Breakfast Seminar(s), see pg 16
Tosoh Bioscience LLC	600		
Trajan Scientific and Medical	702		
Verdel Instruments	314		
VICI	321		
VRS Recruitment	402		
Waters Corporation	300	Marquette Ballroom I-III, VII-IX	Breakfast Seminar(s), see pg 16
Wiley	225		
XP Power LLC	607		
Zef Scientific, Inc.	712		

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!

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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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Mowei Zhou
Ying Zhu

SATURDAY

9:00 AM - 5:00 PM	**SHORT COURSES**

SUNDAY

9:00 AM - 4:30 PM	**SHORT COURSES**
10:00 AM - 8:00 PM	**ATTENTION: FIRST-TIME GRADUATE STUDENTS AND UNDERGRADUATE STUDENTS** **Plan your Strategy: What to See and Do at ASMS,** Hall A
5:00 - 5:45 PM	**TUTORIAL SESSION I,** Hall A **5:00 – 5:45 pm** Mass Spectrometry in Biopharma: From Small Molecules to Multi-Specific Antibodies and Beyond  **Iain D. G.** Campuzano *Amgen Research* **5:45 – 6:30 pm** Machine Learning in Mass Spectrometry  **Randy Julian** *Indigo BioAutomation* **TUTORIAL SESSION II,** Room L100 **5:00 – 5:45 pm** Radical Chemistry for Biomolecular Identification: From Fundamentals to Applications  **Ryan R. Julian** *University of California, Riverside* **5:45 – 6:30 pm** Mass Spectrometry in Natural Product Research  **Laura Sanchez** *University of California, Santa Cruz*
6:45 - 7:45 PM	**CONFERENCE OPENING PLENARY,** Hall A **Julia Laskin**, *Purdue University* ASMS Vice President for Programs **7:00 - 7:45 pm**  Of Stem Cells, Niches and Networks **Judith Kimble** *University of Wisconsin-Madison*
7:45 - 9:00 PM	**WELCOME RECEPTION,** Halls BC All are invited to join us for a festive opening to the conference featuring Corporate Member exhibits. Reception includes display and judging for the Undergraduate Student Poster Competition.

Consult online planner or mobile app for detailed program.

MONDAY

7:00 AM	**Corporate Breakfast Seminars,** Convention Center and Hilton Minneapolis
8:30 - 10:30 AM	**Oral Sessions** MOA am: Post-translational Modifications: Qualitative & Quantitative Analysis, *Hall A* MOB am: Instrumentation: High-Resolution Mass Spectrometry, *Room L100* MOC am: Clinical Analysis: Applications, *Ballroom A* MOD am: Informatics: Multiomics Integration and Applications, *Ballroom B* MOE am: Fundamentals: Formation and Structures of Big Ions, *Auditorium* MOF am: Ion Mobility: Structure Determination & Applications, *Room 101* MOG am: H/D Exchange: Innovations and Applications, *Room 102* MOH am: Plants and Natural Products, *Room 103*
10:30 AM - 2:30 PM	**Poster Session and Exhibits,** Monday Posters, *Hall BC* **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 PM	**Oral Sessions** MOA pm: Biomarkers: Quantitative Analysis, *Hall A* MOB pm: Instrumentation: New Developments in Ionization and Sampling, *Room L100* MOC pm: Drug Metabolism and Pharmacokinetics, *Ballroom A* MOD pm: Informatics: Peptide and Protein Identification, Proteomics, *Ballroom B* MOE pm: Fundamentals of Ionization, *Auditorium* MOF pm: Brain and Neurodegenerative Disease Research (in Memory of Sanford 'Sandy' P. Markey), *Room 101* MOG pm: Exposomics, Toxicology, and Health Outcomes, *Room 102* MOH pm: Environmental: Non-Target Analysis and Emerging Contaminants, *Room 103*
4:45 - 5:30 PM	**Award Lecture,** Hall A  **John B. Fenn Award for a Distinguished Contribution in Mass Spectrometry** preceded by Al Yergey MS Scientist Awards Presentations **Evan R. Williams** *University of California, Berkeley*
5:45 - 7:00 PM	**Workshops** There are light refreshments in foyers, 5:30 - 5:45 pm. 01 Machine Learning: How is it Enhancing Mass Spectrometry? (Independent), *Room L100* 02 Trans-Proteomic Pipeline: Recent Advances and Future Directions (Independent), *Room M100 BC* 03 Incorporating Hands-on Tutorials into Undergraduate Curriculum (Interest Group: Undergraduate Research in MS), *Room M100 DE* 04 Botanical Dietary Supplements: How mass spectrometry is impacting the assessment of the quality (Interest Group: Pharmaceuticals), *Room M100 FG* 05 Molecular Coverage in Ambient Ionization (Interest Group: Ambient Sampling & Ionization), *Ballroom A* 06 Recent development and ongoing challenges with HDX/CL/XL (Interest Group: HDX Covalent Labeling & Cross Linking), *Auditorium Main* 07 Ensuring QA/QC through the Harmonization of Microsampling Techniques in Clinical Chemistry Applications (Interest Group: Clinical Chemistry), *Auditorium Room 1* 08 The NIH and NSF Review and Funding Process (Independent), *Auditorium Room 2* 09 Mass Spectral Libraries: Current and Future Applications (Independent), *Auditorium Room 3* 10 Networking for Scientists: Celebrating Women Mass Spectrometrists (Independent), *Room 101* 11 Career Opportunities for Chinese Students and Scholars (Independent), *Room 102* 12 Real-time Mass Spectrometry in Proteomics and Beyond (Independent), *Room 103* 13 Developing World Outreach (Interest Group: Developing World Outreach), *Room 200 BC* 14 FTMS: FAIR Data for the Masses (Interest Group: FTMS), *Room 200 DE* 15 Polymeric Materials: Coupling of Thermal Polymer Analysis Techniques to MS (Interest Group: Polymeric Materials), *Room 200 FG* 16 The Exposome, Success Stories and the Way Forward (Interest Group: Exposomics), *Room 200 HI*
7:00 - 8:00 PM	**Special Gap Hour Reception sponsored by Agilent,** Room 101 Reception immediately following the Celebrating Women Mass Spectrometrists evening workshop (see 10 above). All are welcome to attend. The goal is to foster networking among the FeMS community and their supporters.
After 8:00 PM	**Corporate Hospitality Suites at Hilton Minneapolis**

TUESDAY

7:00 AM	**Corporate Breakfast Seminars,** Convention Center and Hilton Minneapolis
8:30 - 10:30 AM	**Oral Sessions** TOA am: Biomarkers: Qualitative Analysis, *Hall A* TOB am: Instrumentation: Ionization and Detection of High-Mass Analytes, *Room L100* TOC am: Metabolomics: New Technologies and Applications, *Ballroom A* TOD am: Challenges in MS Analysis of Complex Mixtures, *Ballroom B* TOE am: Fundamentals: Reactions of Gaseous and Solvated Ions, *Auditorium* TOF am: Quantitative Proteomics in Systems Biology, *Room 101* TOG am: GC/MS: Instrumentation and Applications, *Room 102* TOH am: Imaging: Spatially-Resolved Omics, *Room 103*
10:30 AM - 2:30 PM	**Poster Session and Exhibits,** Tuesday Posters, Halls BC **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** TOA pm: Glycopeptides and Glycoproteins, *Hall A* TOB pm: Instrumentation: New Hybrid and Multimodal Approaches, *Room L100* TOC pm: Drug Discovery and Development: Qualitative and Quantitative Analysis, *Ballroom A* TOD pm: Artificial Intelligence in MS Instrumentation and Applications, *Ballroom B* TOE pm: Fundamentals: Ion Activation and Dissociation, *Auditorium* TOF pm: Lipidomics: New MS Technologies and Applications, *Room 101* TOG pm: Stable Isotope Labeling: Applications, *Room 102* TOH pm: Industry: Trace Analysis, Quality Control, and Automation, *Room 103*
4:45 - 5:30 PM	**Award Lecture,** Ballroom B  **Biemann Medal Lecture** preceded by **Research Award Presentations** **Erin Baker** *North Carolina State University*
5:45 - 7:00 PM	**Workshops** There are light refreshments in foyers, 5:30 - 5:45 pm. 01 Big Data Analytics for Energy, Petroleum and Biofuels. (Interest Group: Energy Petroleum & Biofuels), *Room L100* 02 Best Practices for Maintaining Research Continuity in the Shared Resource Laboratory (Interest Group: Analytical Lab Managers), *Room M100 BC* 03 Ion traps and other Technologies that Brought Miniature Mass Spectrometers Mainstream (Interest Group: Ion Trap MS), *Room M100 DE* 04 From Academia to Industry: How Native MS works with complementary technologies to elucidate protein structure. (Interest Group: Native Mass Spectrometry), *Room M100 FG* 05 Reward Those Who Step Up: Helping to Prevent the Burnout of Underrepresented Groups in the Rollout of DEI Activities (ASMS Diversity & Inclusion Committee), *Ballroom A* 06 Isotopes - the Curse and Blessing of Mass Spectrometry (Interest Group: Fundamentals), *Ballroom B* 07 Utilizing GC/MS and Peripheral Technologies for Problem Solving in the Development of FFF Products (Interest Group: Flavor Frangrance & Foodstuff), *Auditorium Main* 08 Extractable and Leachable Testing in Pharmaceutical Industry (Independent), *Auditorium Room 1* 09 Top-Down Mass Spectrometry: Panel Discussion to Address the Community's Challenges (Interest Group: Top-Down Proteomics), *Auditorium Room 2* 10 Kahoot LC-MS Trivia! Stress free fun about LC-MS, ASMS, and Minneapolis! (Interest Group: LCMS & Related Topics), *Auditorium Room 3* 11 How to Kick Start Your Career in Academic or National/Federal Labs (part 1) (Interest Group: Young Mass Spectrometrists), *Room 101* 12 Imaging MS: Opportunities for Artificial Intelligence and Machine Learning (Interest Group: Imaging MS), *Room 102* 13 Towards probability-based metabolite identification confidence (Independent), *Room 103* 14 HUPO Proteomics Standards Initiative and ProteomeXchange for FAIR Biological MS (Independent), *Room 200 BC* 15 Photoionization MS: How to Identify the Best Technique for an Analytical Problem? (Interest Group: Photoionization MS), *Room 200 DE* 16 Recent Advances in ADME Biomarkers (Interest Group: DMPK), *Room 200 FG* 17 Visualization of Mass Spectrometry related data (Interest Group: Bioinformatics MS), *Room 200 HI*
7:00 - 8:00 PM	**Special Gap Hour Reception sponsored by MOBILON,** Ballrom A Reception immediately following the ASMS Diversity & Inclusion Committee's evening workshop (see 05 above). All are welcome to attend. The goal is to foster networking among those interested in issues of diversity and inclusion.
After 8:00 PM	**Corporate Hospitality Suites at Hilton Minneapolis**

WEDNESDAY

7:00 AM	**Corporate Breakfast Seminars,** Convention Center and Hilton Minneapolis
8:30 - 10:30 AM	**Oral Sessions** WOA am: Biotherapeutics: Proteins, Antibodies, and Antibody/Drug Conjugates, *Hall A* WOB am: Instrumentation: Innovative Separations Approaches Coupled to MS, *Room L100* WOC am: Imaging: Pharmaceuticals, Metabolites, Lipids, and Glycans, *Ballroom A* WOD am: Informatics: Metabolomics, *Ballroom B* WOE am: Fundamentals: Ion Structures and Energetics (In Memory of Fred W. McLafferty), *Auditorium* WOF am: Lipidomics: Targeted and Untargeted, *Room 101* WOG am: Forensics: Innovations and Applications, *Room 102* WOH am: Environmental: Innovative Approaches and Instrumentation, *Room 103*
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: Biotherapeutics: Characterization and Quantitation, *Hall A* WOB pm: Instrumentation: Ambient Ionization and Applications, *Room L100* WOC pm: Metabolomics: Untargeted Profiling, *Ballroom A* WOD pm: Nucleic Acids and Oligonucleotides, *Ballroom B* WOE pm: Fundamentals Beyond Mass Analysis: Structural Characterization of Isomers, *Auditorium* WOF pm: Protein-Ligand and Protein-Protein Interactions, *Room 101* WOG pm: Microbiome and Interactome, *Room 102* WOH pm: Viruses and Virus-Like Particles, *Room 103*
4:45 - 5:30 PM	**ASMS Meeting,** Hall A. 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 Current Landscape of High Throughput Sample Preparation in Quantitative MS (Independent), *Room L100* 02 Multi-Attribute Method (MAM): New Aspects in Development (Interest Group: Biotherapeutics), *Room M100 BC* 03 Periodic Table of Food Initiative: Engaging the Mass Spectrometry Community in the Development of a Democratized Foodomics Technology Platform (Independent), *Room M100 DE* 04 Recent Advances in Oligonucleotides & Peptides Bioanalysis by Triple Quad and HRMS (Interest Group: Regulated Bioanalysis), *Auditorium Main* 05 Efficient Analysis of Wastewater by Advanced Mass Spectrometry Techniques (Interest Group: Environmental Applications), *Auditorium Room 1* 06 Forensic Mass Spectral Technology: The Transition from Research to Practical Application (Interest Group: Forensics & Homeland Security), *Auditorium Room 2* 07 Data Independent Acquisition Goes Mainstream? (Interest Group: Data Independent Acquisition), *Ballroom A* 08 Single-cell proteomics: From Sample Preparation to Data Analysis (Independent), *Ballroom B* 09 How to Kick Start Your Career in Industry (part 2) (Interest Group: Young Mass Spectrometrists), *Room 101* 10 Cannabis & Hemp Science: The Importance of Mass Spectrometry (Independent), *Room 102* 11 Characterizing Greatness: Celebrating Fred McLafferty (Independent), *Room 103* 12 Democratizing Metabolomics: Lessons learned and future directions from US regional core facilities (Interest Group: Metabolomics), *Room 200 BC* 13 Allyship: Embracing Diversity and Inclusion in Your Workplace (Interest Group: Career Development), *Room 200 DE* 14 Cloud Resources for Proteomics Analysis (Independent), *Room 200 FG* 15 Ion Mobility Spectrometry: What's next? (Interest Group: Ion Mobility MS), *Room 200 HI*
After 8:00 PM	**Corporate Hospitality Suites at Hilton Minneapolis**

Consult online planner or mobile app for detailed program.

THURSDAY

7:00 AM	**Corporate Breakfast Seminars,** Convention Center and Hilton Minneapolis
8:30 - 10:30 AM	**Oral Sessions** ThOA am: Structural Biology, *Hall A* ThOB am: Ion Mobility: Instrumentation & Method Development, *Room L100* ThOC am: Single Cell Omics, *Ballroom A* ThOD am: Informatics: Data-Independent Acquisition and Multiplexing, *Ballroom B* ThOE am: Fundamentals: Unconventional Approaches in MS (Honoring R. Graham Cooks), *Auditorium* ThOF am: Cancer Research, *Room 101* ThOG am: Food Safety & Chemistry: Innovations, *Room 102* ThOH am: High Throughput MS, *Room 103*
10:30 AM - 2:30 PM	**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 PM	**Oral Sessions** ThOA pm: Top Down Protein Analysis, *Hall A* ThOB pm: Imaging: Instrumentation & Method Development, *Room L100* ThOC pm: Clinical Analysis: Innovations, *Ballroom A* ThOD pm: Informatics: Innovations, *Ballroom B* ThOE pm: Covalent Labeling and Chemical Crosslinking, *Auditorium* ThOF pm: Glycomics, *Room 101* ThOG pm: Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, and Supplements, *Room 102* ThOH pm: Small Molecules: Structural Characterization and Quantitation, *Room 103*
4:45 - 5:30 PM	**Plenary Lecture,** Hall A  *Homo naledi* and the Chamber of Secrets **Jeremy DeSilva** *Dartmouth College*
6:30 – 10:30 PM	**Closing Event: Dinner & PurpleXperience Concert,** Hall D Advance Purchase Ticket Required, Sales close at 12pm noon MONDAY (June 6). Purchase your ticket online via Registration portal.

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

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

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

TUESDAY 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

Consult online planner or mobile app for detailed program.

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

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

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

All evening workshops are 5:45 – 7:00 pm. There are light refreshments in the foyers, 5:30-5:45 pm.

MONDAY WORKSHOPS

01 Machine Learning: How is it Enhancing Mass Spectrometry? (Independent)

Presiding: Gaurav Chopra, Kevin Bateman, Shane Tichy

Room L100

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 questions 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 ion-molecule 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.

02 Trans-Proteomic Pipeline: Recent Advances and Future Directions (Independent)

Presiding: Eric Deutsch, Luis Mendoza

Room M100 BC

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 6.1.0 release, including:

- Deploying Enterprise TPP for the whole lab on your local computing cluster
- Deploying TPP using Docker or AWS/Azure cloud computing services
- PTMProphet analysis of Magnum open-mass search results
- Using entrapment database searching for proteomics MS analysis

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

03 Incorporating Hands-on Tutorials into Undergraduate Curriculum (Interest Group: Undergraduate Research in MS)

Presiding: Patrick Fedrick, Hannah M. Brown, Nicolas Mauricio Morato Gutierrez, Mac Gilliland, Christine Hughey, and Brandie M. Ehrmann

Room M100 DE

Undergraduate exposure to hands-on experience in mass spectrometry is typically very limited. Barriers to such experiences can be multi-faceted, but an argument could be made that the single largest factor is limited physical access to instrumentation. Second to that is the lack of dedicated undergraduate coursework in mass spectrometry. Panelist in this workshop aim to explore how PUIs and R1 institutions are working to overcome these limitations by incorporating hands-on MS tutorials into the undergraduate curriculum. Dedicated conversation about overcoming barriers that inhibit or discourage implementation of practical mass spectrometry teaching laboratories will be a major topic of discussion. Real-world applicability of mass spectrometry-based experimentation will serve as a guiding principle in the design of these tutorials; helping reinforce the importance of this analytical tool for undergraduates.
Special attention will be given to how the MS community could potentially share basic data sets to enable exposure and facilitate undergraduates working through mass spectrometry data analysis. Improve accessibility to software and/or freeware that can be utilized to help interpret spectra will also be examined. Attendees of this workshop should expect a highly interactive environment that will incorporate input from participants to generate a practical, workable, and tractable solution for an improved hands-on approach to teaching mass spectrometry at the undergraduate level at both PUIs and R1 institutions.

04 Botanical Dietary Supplements: How mass spectrometry is impacting the assessment of the quality (Interest Group: Pharmaceuticals)

Presiding: Angela Calderon, Kiran Iyer

Room M100 FG

The botanical dietary supplements (BDS) are complex mixtures of natural products with health benefits. This type of dietary supplement is popular among the US population. Their consumption has increased during the pandemic to enhance the immune response. The increasing popularity of these products has generated an increase in adulteration and low quality in these DS. State-of-the-art techniques such as LC-MS with high resolution and sensitivity are necessary to address the quality of the complex BDS. The good quality of these DS will assure their efficacy and safety in humans. Traditionally, the evaluation of the quality of BDS is carried out with thin layer chromatography and LC-UV. This workshop aims to present 1) the status on the use of LC-MS for analysis of BDS, 2) the perspective on the introduction of LC-MS to monographs of quality by United States Pharmacopeia (USP), and 3) more suitable LC-MS for the quality assessment of these products presented by Agilent, Waters, and Thermo. The order of the presentations will be topic

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MONDAY WORKSHOPS

1 by presider 1, topic 2 by a representative of USP, and topic 3 by a representative of each LC-MS company Agilent, Waters, and Thermo. The audience for the workshop will be the industry community, researchers in academia, and analytical contract laboratories. Appropriate time will be destinated to encourage participation and idea exchange with the audience. An expected outcome is to trigger the interest in the industry to embrace LC-MS's capabilities to assure the quality of BDS.

05 Molecular Coverage in Ambient Ionization (Interest Group: Ambient Sampling & Ionization)

Presiding: German Gomez-Rios, G. Asher Newsome, Anyin Li

Ballroom A

A wide variety of ion sources using different physical and chemical processes fall under the umbrella term of "ambient sampling and ionization" - but not every source can analyze every compound. Following the list of top concerns as voted in 2019, we will convene a panel to discuss molecular coverage in a world of unknown samples, limited budgets, and finite time to optimize methods for a given analyte. Discussion is expected to range from advantages and pitfalls of certain techniques to the mythical (but no less desirable) ion source that Does It All. The panel Q&A will be preceded by several 3-minute lightning talks selected from 2022 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.

06 Recent development and ongoing challenges with HDX/CL/XL (Interest Group: HDX Covalent Labeling & Cross Linking)

Presiding: Miklos Guttman, Corie Ralston, Clinton Yu

Auditorium Main

Developments in MS instrumentation, sample preparation strategies, reagents and informatics tools have significantly advanced applications of HDX, covalent labeling and cross-linking approaches in protein structural and interaction analysis. This workshop will give the researchers a chance to discuss recent developments and ongoing challenges related to each of these methods. Various experts from each discipline will be present to contribute to the discussion.

07 Ensuring QA/QC through the Harmonization of Microsampling Techniques in Clinical Chemistry Applications (Interest Group: Clinical Chemistry)

Presiding: Candice Ulmer, Don Chace

Auditorium Room 1

The integration of dried blood spots (DBS) and mass spectrometric analyses in clinical chemistry originated in the newborn screening field more than 30 years ago. Currently, newborn screening tests using DBS and MS/MS are routinely performed worldwide with many millions of infants being screened annually. Early laboratory screening programs in NC and PA quickly recognized the importance of standardization in ensuring the accuracy of reported clinical measurements. Acknowledging this need, the Newborn Screening and Molecular Biology Branch of the Centers for Disease Control developed the Newborn Screening Quality Assurance Program, which not only develops newborn screening MS/MS methods for the DBS measurement of clinical markers, but also provides QC materials and proficiency testing. This program alongside other international groups in Europe and Australia/New Zealand ensure the harmonization of newborn screening tests.

Advancements in microsampling, the capture of less than 100 µL, have allowed for the expansion of clinical applications beyond newborn screening such as the use of DBS in COVID-19 testing. Microsampling techniques now have the advantage of reduced shipping and storage costs, reduced infectious disease exposure, and remote specimen collection. However, the need for standardization has become even more important with this increased interest in microsampling techniques and the emergence of collection devices beyond the filter paper (Guthrie) card. This workshop will discuss the advantages/disadvantages of microsampling techniques compared to venous blood draws, new approaches to improving the MS quantification of clinical measurements to make MS analysis more amenable to clinical chemistry applications, and existing microsampling QA/QC standardization programs.

08 The NIH and NSF Review and Funding Process (Independent)

Presiding: Salvatore Sechi, Kelsey Cook, Douglas Sheeley, and Kenneth Ryan

Auditorium Room 2

Many ASMS members and conference participants are supported by the National Institutes of Health and 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 NIH and NSF 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.

09 Mass Spectral Libraries: Current and Future Applications (Independent)

Presiding: Lewis Geer, Melinda McFarland, Douglas Slotta

Auditorium Room 3

Mass spectral (MS) libraries find wide applicability in areas of science that employ mass spectrometers to precisely identify molecules. This workshop will provide a forum to update participants on the latest developments and uses of MS libraries and to discuss future needs and applications of these resources. A panel of experts will present state-of-the-art applications of spectral libraries, including use in pharma and environmental studies. They will also provide their expert opinions on the new directions MS libraries may take. Their presentations will be followed by an extended Q&A period and a panel discussion based on questions of general interest to the audience. Topics

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MONDAY WORKSHOPS

may include the use of LC-MS/MS and GC-MS libraries in data independent acquisition and other (glyco)proteomics methods, metabolomics, food and fragrances, lipidomics, environmental analysis, forensics, and software tool development, including searching. The discussion will include the potential use of libraries in new technologies, like electron impact excitation of ions from organics (EIEIO). Groups that create spectral libraries as well as scientists that use them are invited. Our end goal is to inform participants of the capabilities of MS libraries and instigate discussions that may lead to improvements in the creation and usage of existing libraries, as well as new avenues of research.

10 Networking for Scientists: Celebrating Women Mass Spectrometrists (Independent)

Presiding: Molly Soper-Hopper, Komal Kedia, Aivett Bilbao

Room 101

Building off previous 5 years of the Celebrating Women Mass Spectrometrists workshops, this year a panel of ~3 mass spectrometrists will discuss how they navigated big career changes. Panelists will come from different backgrounds including (but not limited to) parents, LGBTQIA+, minority people groups, international workers, and disabled individuals. We will explore a broad definition of "career change" which includes what considerations a woman might make as early as graduate school through advanced career stages. Topics may include moving long distances/internationally for a postdoc or permanent position, moving a family or pausing a career to care for children and the two-body problem, transitions from academia to industry (including graduation) and vice versa, knowing when to move to a new company for better work-life balance, adapting to the culture of a new workplace especially for individuals in a minority, how advocate for/take/decline promotions, and others as questions arise from attendees. As in years past, panelists will be introduced and then take time to discuss career paths they have followed, what factors they considered when making big decisions, and advice they would give to a woman facing the same challenges. We will leave time for questions and networking for more personalized interactions.

11 Career Opportunities for Chinese Students and Scholars (Independent)

Presiding: Junmin Peng, Shuguang Ma

Room 102

With the rapid development of mass spectrometry technologies and the increasing applications to academic research, medicine, industry, and regulatory agencies, a growing number of mass spectrometrists including thousands of Chinese students and scholars are trained. The workshop for Career Development Opportunities for Chinese Students and Scholars aims to provide career perspectives to students and scholars to learn the career paths at different career stages. We will invite four speakers from academia, clinic, industry, and regulatory agencies to share their experiences for career development. We will also assemble a group of discussion panelists to answer questions from the audience. We believe the workshop is beneficial to both students and scholars of all ASMS members and potential employers. The workshop will provide opportunities for students and scholars to prepare for their career development during and after mass spectrometry training and help them to set up career goals in the field of mass spectrometry.

12 Real-time Mass Spectrometry in Proteomics and Beyond (Independent)

Presiding: Christopher Adams, Devin Schweppe, Mathieu Lavallee

Room 103

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 real-time 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.

13 Developing World Outreach (Interest Group: Developing World Outreach)

Presiding: Kym Faull, Giles Edwards, Hendrik Kersten

Room 200 BC

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 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.

14 FTMS: FAIR Data for the Masses (Interest Group: FTMS)

Presiding: Chad Weisbrod, David Butcher

Room 200 DE

Findability, accessibility, interoperability, and reusability are the principles which define FAIR data and the greater movement towards making scientific data reusable by both humans and machines. The FAIR data movement is currently a high priority initiative for funding agencies (e.g. NSF, NIH, DOE) and many journal publishers and increasingly, mass spectrometrists will be asked to make their data FAIR by imposition of policies by these groups. Fortunately, there are a plethora of benefits to be gained from making data FAIR. During this workshop, we intend to introduce FAIR data as it relates to mass spectrometry

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MONDAY WORKSHOPS

and FTMS. We'll discuss the implications of making FTMS data FAIR for different types of applications (biological, complex mixtures, MS imaging) and the benefits to be gained. There will be speakers invited covering a range of FAIR related topics. Attendees will have the opportunity to ask questions and participate in a round table discussion. The aim is to help ease those folks into transitioning into a FAIR data ecosystem and discuss progress in making our facility at the National MagLab FAIR compliant.

15 Polymeric Materials: Coupling of Thermal Polymer Analysis Techniques to MS (Interest Group: Polymeric Materials)

Presiding: Jessica Hoskins, Thierry Fouquet

Room 200 FG

This year's workshop will consist of three distinct sections: a tutorial discussion, poster elevator talks, and an open forum.
To being, we will host a short tutorial session on the coupling of thermal polymer analysis techniques with MS. This topic was chosen based on feedback from the interest group and is intended to encourage interactive discussion. Second, we will host a series of short (1-2 min each) promotions of polymer related posters open to any presenters who wish to highlight their work to the interest group's specialized audience.

The workshop will conclude with an open forum in which attendees are invited to bring forward polymer related issues or questions they would like help with. The discussion will conclude with suggestions for future workshop topics and other administrative items.

16 The Exposome, Success Stories and the Way Forward (Interest Group: Exposomics)

Presiding: Silvia Balbo, Benedikt Warth

Room 200 HI

The workshop will inform and discuss the latest developments in the expanding field of exposome research. An overview on the latest developments in the field together with a number of recent "success" stories will be presented. This includes work from a number of renowned labs working in the area. Future directions of exposomics will be discussed in light of a massive push coming from both, US-based and European initiatives leading the way toward innovative and multidisciplinary research in the arena of environmental health and personalized prevention.

TUESDAY WORKSHOPS

01 Big Data Analytics for Energy, Petroleum and Biofuels (Interest Group: Energy Petroleum & Biofuels)

Presiding: Leonard Nyadong, Yuri Corilo

Room L100

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 spectrometry-based 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 data FAIR and accessible; (3) Maintaining quality data; and (4) Keeping data secure; and (5) ensuring metadata capture required for each sample type.

02 Best Practices for Maintaining Research Continuity in the Shared Resource Laboratory (Interest Group: Analytical Lab Managers)

Presiding: Brett Phinney, Ryan Leib, Alexandre Rosa Campos, and Joanna Kirkpatrick

Room M100 BC

An opportunity to share best practices for maintaining core competencies and research continuity across personnel changes. The session will focus on sharing strategies, tools, and practical tips for maintaining scientific continuity as personnel changes naturally occur in a shared resource facility and its users. Come prepared to participate and engage with your fellow lab managers.

03 Ion traps and other Technologies that Brought Miniature Mass Spectrometers Mainstream (Interest Group: Ion Trap MS)

Presiding: Theresa Evans-Nguyen, Dalton Snyder

Room M100 DE

"Looks like we made it" by American singer Barry Manilow reached the #1 spot on the US Billboard Hot 100 in 1977. Four and a half decades later, the title of the song is an apt summary of the progress that the field of miniature and portable mass spectrometry has made in the 21st century. Despite enormous technological challenges, namely maintaining system performance while necessitating reductions in system size, weight, and power (SWaP), and notable disinterest from many in the MS community throughout the early years, miniature mass spectrometers have 'made it' commercially and are set to revolutionize chemical analyses in the field.

All evening workshops are 5:45 – 7:00 pm. There are light refreshments in the foyers, 5:30-5:45 pm.

TUESDAY WORKSHOPS

In this workshop the ion trap interest group will first hear brief (~5 min) presentations from several pioneers in the miniature MS community, namely prominent scientists from small and large instrument vendors, universities, and government laboratories, who will be invited to discuss the enabling technologies critical to the success of the instruments that 'made it' to commercialization. The topics are expected to be wide-ranging, from miniaturization of mass analyzers (particularly ion traps) to development of novel approaches for sampling, ionization, ion transport, and power and vacuum management. Unlike previous workshops, emphasis will be placed on late-stage technologies rather than early-stage or theoretical developments to broaden the appeal compared to prior years. Presenters will be encouraged to be interactive and to bring MS components with them for audience perusal. The evening will conclude with a roundtable discussion of the current state and future of the field.

04 From Academia to Industry: How Native MS works with complementary technologies to elucidate protein structure. (Interest Group: Native Mass Spectrometry)

Presiding: Elizabeth Hecht, Ashley Bell, Justin Benesch

Room M100 FG

Native MS is recognized as a cutting edge technique in the molecular characterization of protein targets and drugs. It can provide information regarding complex stoichiometry, structural integrity, noncovalent ligands, drug binders, and post-translational modifications. As research targets in academics and industry become more challenging, there is an increasing need to integrate native MS with other orthogonal technologies to solve structures at hand.

The last two years have witnessed a growth in complementary technologies or methodologies to native MS to assist in structural characterization. Exciting developments have been made in soft landing (interface of microscopy and native MS), binding interface elucidation (interface of cross-linking and native MS), and stoichiometry (interface of mass photometry, ion mobility, and native MS). This workshop will highlight the integration of traditional native mass spectrometry structural biology with these emerging complementary technologies. For newcomers to the field, the workshop will also seek to address which routine instrumentation may be desirable for inclusion in a new native MS lab looking toward structural characterization.

The native MS workshop has long supported collaboration between academia and industry. The panel of experts will sit on both sides, presenting work that is cutting-edge both in technique and application area. The workshop will deliver short lightning talks followed by a facilitated discussion.

05 Reward Those Who Step Up: Helping to Prevent the Burnout of Underrepresented Groups in the Rollout of DEI Activities (ASMS Diversity & Inclusion Committee)

Presiding: Jennifer Campbell, Saiful Chowdhury, Carlos Larriba-Andaluz, Dominic Gostick, Candice Ulmer, Richard Yost

Ballroom A

Many workplaces and laboratories have committed to eliminate barriers associated with job opportunity and professional development equity, establish more inclusive and accessible environments, and improve the success/retention of individuals from underrepresented and/or underserved groups. As a result, scientists have witnessed the birth of internal diversity, equity, inclusion, and accessibility (DEIA) strategic plans, mandatory training modules, DEI task groups, and other activities. However, these roles are often disproportionally filled internally by scientists from the same underrepresented groups that the DEI initiatives were intended to benefit (e.g., womxn and minorities), added on top of their normal workloads, and accepted with no added incentives, benefits, and/or recognition. Therefore, this workshop will provoke a discussion on best practices and effective strategies to mitigate the burnout of underrepresented groups in the rollout of DEI work.

06 Isotopes - the Curse and Blessing of Mass Spectrometry (Interest Group: Fundamentals)

Presiding: Alexander Makarov, Alexandre Shvartsburg

Ballroom B

Since Aston discovered isotopes using mass spectrometry a century ago, the two fields have been intertwined. The omnipresence of isotopes has powerfully driven the technology development in mass analyzers, detectors, and data processing, enabled novel analyses in areas ranging from climate research to metabolic tracing in fluxomics, and penetrated numerous MS applications. The first major industrial employment of MS was preparative separation of uranium isotopes in the Manhattan project. Today, stable isotope labeling underlies most chemical quantification methods. A unique but crucial capability is the carbon-14 dating via accelerator MS. Of recent novelty is the emergence of isotopic effects in ion mobility separations (IMS) and initial exploration of their magnitude, mechanism, and utility. The presence and use of isotopes remains a rare common aspect across the vastness of modern MS universe.

This workshop will involve speakers from diverse research areas united by the passion for isotope measurements and their use to advance the frontier of analytical science.

We tentatively plan the presentations by:

- Thomas Angel (GSK) or Sasha Singh (Boston): Isotopes and HR MS in fluxomics
- John Eiler (Caltech): Position- and bond- selective isotope ratio measurements of organic molecules
- Roman Zubarev (Karolinska): Isotope resonance and abnormalities in nature discovered using proteomics or top-down analyses of isotopically depleted proteins
- Rosa Viner (Thermo Fisher): Isotopes for multiplexing (TMT, iTRAQ, next)
- Alexandre Shvartsburg (Wichita State): Structural isotopic effects in IMS
- An FTMS user: Compound disambiguation exploiting fine isotopic structure

07 Utilizing GC/MS and Peripheral Technologies for Problem Solving in the Development of FFF Products (Interest Group: Flavor Frangrance & Foodstuff)

Presiding: Travis Falconer, Joe Binkley

Auditorium Main

There are numerous challenges that may arise throughout the course of developing flavor, fragrance, and foodstuff (FFF) products. Due to the nature of many of the molecules

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TUESDAY WORKSHOPS

responsible for a product's flavor and fragrance profile, GC/MS is frequently the tool of choice for tackling these challenges. There may be projects for which the standard workhorse GC-quadrupole MS system is sufficient, but there are now many commercially available variations, which employ advanced multi-dimensional separations, time-of-flight, triple-quadrupole, and/or high-resolution mass spectrometers, as well as various peripherals such as olfactory detection for those projects that require them.

The goal of this workshop is to enhance attendees' knowledge about how various GC/MS systems may be used to tackle problems throughout the development cycle of FFF products. Several applications utilizing GC/MS and peripheral technologies will be described, which will serve as a starting point for a group discussion intended to engage and benefit attendees.

The workshop format will consist of two parts: 1) Several panelists will provide brief examples of problems that have been solved in the development of FFF products using GC/MS and peripheral technologies. 2) Interactive discussion among attendees and panelists moderated by the interest group co-chairs, including engagement with attendees by interactive, smartphone-based polling.

08 Extractable and Leachable Testing in Pharmaceutical Industry (Independent)

Presiding: Gyorgy Vas, Katie Comstock

Auditorium Room 1

Extractable and leachable testing is one of the concerning issue for today's FDA submissions. It is a critical part for the toxicological safety risk assessment for small molecule and biology based drug products as medical devices. Recent issues in the industry related to trace level impurities in finished pharmaceutical and consumer products further highlights the importance of E&L testing (nitrosamine, benzene). Additionally emerging impurities such as polyfluorinated hydrocarbons may needed to be evaluated in medical devices. The workshop will discuss different testing approaches, identification and quantitation of unknowns and progress of use component databases.

09 Top-Down Mass Spectrometry: Panel Discussion to Address the Community's Challenges (Interest Group: Top-Down Proteomics)

Presiding: Caroline DeHart, Mowei Zhou

Auditorium Room 2

Top-down mass spectrometry (TDMS) can provide molecular details at the intact protein level inaccessible by conventional proteomic approaches. However, TDMS sample preparation, instrumentation, and data analysis methods are not yet as robust as the widely adopted bottom-up proteomics methods. These unique challenges can be particularly prohibitive to new or novice practitioners. In this workshop, we will feature a panel comprising representatives from academia, government, industry, and startup laboratories. This panel will lead a lively and engaging discussion with audience members either currently employing or interested in applying TDMS methods to their ongoing research objectives. Primary topics of discussion will include: 1) What has and has not been going well for TDMS adoption by newcomers; 2) New resources (e.g., databases, webinars, tutorials) needed for easier TDMS adoption; 3) New areas that could greatly benefit from application of TDMS; and 4) New technical developments in TDMS required to successfully tackle current challenges. The panel will address each topic in turn, followed by live questions from the audience to facilitate further discourse. At the conclusion of the panel discussion, members of the executive board of the Consortium for Top-Down Proteomics will be invited to respond to the points raised and engage the audience in planning how to broaden adoption of TDMS across the greater research community. Contact workshop chairs with suggested questions for the panel or to apply for the 2023 workshop co-chair position.

10 Kahoot LC-MS Trivia! Stress free fun about LC-MS, ASMS, and Minneapolis! (Interest Group: LCMS & Related Topics)

Presiding: James Dodds, Jack Ryan, Michael Doyle

Auditorium Room 3

Do you love trivia and want a chance to kick back and take it easy? Let's be honest. ASMS can be overwhelming! So much good science to take in but with all the posters, talks, meetings and workshops to go to ASMS is a crazy week! Why not sit back, relax, crack open a free beverage, and enjoy your evening with some fun trivia about LC-MS topics, ASMS, and random facts about Minneapolis!

The game will be played over the easy-to-use phone app called Kahoot, where everyone will answer multiple choice and matching questions and your score is calculated on 1) right answers and 2) the speed at which you answer the question. You'll be competing against others at the conference and attendees from home, so bring your A game! We'd love to have you in person for this workshop, but if you're attending ASMS from home logging in and joining the fun is super easy.
Looking forward to seeing you in the Twin Cities, and best wishes!

11 How to Kick Start Your Career in Academic or National/ Federal Labs (Part 1) (Interest Group: Young Mass Spectrometrists)

Presiding: Laura Sanchez, Chris Pulliam

Room 101

The Young Mass Spectrometrists workshop part 1 will focus on a panel discussion where representatives from academia, government, and national labs will discuss aspects of their personal journeys and opportunities that highlight not only how to break into this sector but also challenges and benefits to these positions. Through this discussion mass spectrometrists at the undergrad, graduate, or postdoctoral stage of their career learn information and strategies that will help them navigate the next steps in their career. This panel will be composed of representatives from academia, federal, and government career paths to provide a targeted discussion of these types of career opportunities for young researchers who have mass spectrometry skills. Time permitting and level of interest, 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.

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12 Imaging MS: Opportunities for Artificial Intelligence and Machine Learning (Interest Group: Imaging MS)

Presiding: Alison Scott, Ingela Lanekoff

Room 102

Background and Focus:
Artificial Intelligence (AI) and Machine Learning (ML) methods are maturing in parallel with spatially resolved, 'omics- scale mass spectrometry applications. A growing number of computational experts are working with imaging mass spectrometry data, and through this work, experimental conclusions and new information embedded in a dataset can be explored and unlocked. Impressive strides are made in this area each year. Yet, few tools exist to apply AI and ML to imaging mass spectrometry that function at an accessible level for a non-computational scientist. This workshop aims to discuss the current state of the field, identify accessible tools and software, best practices and pinpoint hurdles to the broad uptake of AI and ML tools for imaging mass spectrometry analysis.

Organization:
This workshop will be presented in two parts. First, an invited speaker will briefly present current background, tools, and hurdles in AI and ML applied to imaging mass spectrometry followed by Q&A. Second, an organized panel discussion will explore the pros and cons of these techniques and address participant questions and challenges. Please come with questions, comments, and discussion topics for the panel and audience.

13 Towards probability-based metabolite identification confidence (Independent)

Presiding: Tom Metz

Room 103

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 an initial conceptual model for assigning a probability to quantify the evidence for the presence of a compound in a sample and that is 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.

14 HUPO Proteomics Standards Initiative and ProteomeXchange for FAIR Biological MS (Independent)

Presiding: David Tabb

Room 200 BC

The Proteomics Standards Initiative (PSI, http://www.psidev.info) and ProteomeXchange (http://www.proteomexchange.org) are two highly collaborative projects that are open to contributions from everyone in the biological MS community. The FAIR principles guide biomedical researchers to responsible and reproducible science, specifying that science data should be Findable, Accessible, Interoperable, and Reusable. This workshop will update the mass spectrometry community on ways that HUPO-PSI and ProteomeXchange are advancing FAIR science through data standards and data communication. The knowledge management infrastructure encompasses the repositories (such as PRIDE, PeptideAtlas, MassIVE, jPOST, iProx and Panorama Public), journal editors, funding bodies, and of course mass spectrometry scientists.

We will briefly showcase our most successful projects and highlight some of our ongoing activities, highlighting current trends in re-use of public proteomics datasets and fostering discussion among participants about what future directions in both initiatives would most benefit the community. Please attend if you want your voice to be heard!

15 Photoionization MS: How to Identify the Best Technique for an Analytical Problem? (Interest Group: Photoionization MS)

Presiding: Christopher Rüger, Matthias Lorenz

Room 200 DE

We reviewed the fundamentals of photoionization (PI) MS in our 2018 workshop and discussed existing techniques as either vacuum or atmospheric pressure-based in 2020. We have therefore decided that this year's PI workshop will address the challenge of identifying the most suitable PI technique for an analytical problem. This topic ties up to the 2019 workshop in which we addressed the transfer of PI techniques from academic research to industrial applications. We are planning this year to discuss the broad variety and complex nature of techniques that define their different experimental requirements and to estimate their analytical potential. Published data often use different mass spectrometers, sample delivery systems, and analytical targets (e.g., molecular vs. elemental species). Furthermore, the light source, PI source design, and mass spectrometer are often either not designed in a modular way and/or cannot be readily moved between different instruments. Three experts in their particular subfields of photoionization MS will present on their respective work to help illustrate the substantial differences between existing techniques beyond just their pressure regimes. This should allow for an energetic discussion while also serving as a broad overview for newcomers to the field.

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16 Recent Advances in ADME Biomarkers (Interest Group: DMPK)

Presiding: Bhagwat Prasad, Lina Luo

Room 200 FG

Drug transporters and metabolizing enzymes are important determinants of drug absorption, metabolism, distribution, and elimination (ADME) and influence drug-drug interactions (DDIs) and toxicity. Recommended, in vitro-determined, DDI risk thresholds for transporters are known to be conservative thus it is not a surprise that, false positive rates are high. While significant progress has been made to utilize in vitro models to predict drug ADME using physiologically-based pharmacokinetic (PBPK) models, PBPK modeling requires comprehensive physiological data on inter-individual variability. Tissue abundance analysis of enzymes and transporters in tissue biopsies or autopsy samples is one of the approaches for assessing the effect of population covariates. However, limited availability and poor quality of tissue samples are the key challenges of this approach to characterize variability in drug disposition. ADME biomarkers that can be quantified using accessible biofluid such as urine and blood from patients or healthy volunteers are recognized as a relatively non-invasive and better approach to facilitate clinical phenotyping and DDI assessment, in conjunction with DDI decision trees from regulatory agencies. For example, coproporphyrin I and III are viable biomarkers of organic anion transporting polypeptides (OATPs) that have been used to predict transporter inhibition and the impact of genetic polymorphism. Recent data on renal organic anion transporters (OATs) in human and preclinical species suggest promising clinical application of these biomarkers in assisting drug development. Such approaches are also emerging for DMEs, both Phase I and Phase II. This workshop will bring together established researchers from the pharma industry and academia to discuss recent advances in ADME biomarkers.

17 Visualization of Mass Spectrometry related data (Interest Group: Bioinformatics MS)

Presiding: Arzu Tugce Guler, Claire O'Donovan

Room 200 HI

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.

All evening workshops are 5:45 – 7:00 pm. There are light refreshments in the foyers, 5:30-5:45 pm.

WEDNESDAY WORKSHOPS

01 Current Landscape of High Throughput Sample Preparation in Quantitative MS (Independent)

Presiding: Pankaj Dwivedi

Room L100

This workshop will provide an open platform to discuss new advances in the high throughput sample preparation for quantitative proteomics-based studies. The workshop will cover the limitations of the current methods and recent improvements showing considerable changes in the overall data quality as well as its implications for the understanding of biology.

Presenters:

1. Nikolai Slavov (Northeastern University), Increasing the throughput of sensitive protein analysis
2. Jakob Vowinckel (Biognosys), Automation in large-scale proteomics: From sample to data without manual intervention
3. Keith Rivera (Broad Institute), UbiFast: an automated workflow for ubiquitin analysis
4. Ryan Bomgarden (Thermo Fisher Scientific), Adapting EasyPepTM MS sample preparation and TMTTM labeling reagents for higher throughput platforms

02 Multi-Attribute Method (MAM): New Aspects in Development (Interest Group: Biotherapeutics)

Presiding: Richard Rogers, Da Ren

Room M100 BC

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 industry-wide 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.

03 Periodic Table of Food Initiative: Engaging the Mass Spectrometry Community in the Development of a Democratized Foodomics Technology Platform (Independent)

Presiding: Jessica Prenni, Steve Watkins, John de la Parra

Room M100 DE

Food is at the center of addressing some of the world's most urgent challenges. However, our scientific understanding of the biochemical composition of food is rudimentary. The Periodic Table of Food Initiative (PTFI) is a global effort focused on the creation of a composition reference database of the food we eat with the goal of revolutionizing human health and sustainable agriculture. Key to this goal is the very challenging task of developing a standardized, fully democratized LC-MS based technology platform for generating comprehensive food composition data. It is envisioned that such a platform could be used by laboratories around the world to populate a reference database that enables comparability of data. The objectives of this workshop will be to: (1) introduce the PTFI to the broader mass spectrometry community; (2) spark innovative ideas and feedback and; (3) discover new opportunities for engagement.

04 Recent Advances in Oligonucleotides & Peptides Bioanalysis by Triple Quad and HRMS (Interest Group: Regulated Bioanalysis)

Presiding: Jian Wang, Dian Su, Wenkui Li

Auditorium Main

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 eight peptides and two oligos in 2021, we are looking forward to seeing expanded interests in medium-size therapeutics. The 2022 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.

05 Efficient Analysis of Wastewater by Advanced Mass Spectrometry Techniques (Interest Group: Environmental Applications)

Presiding: Ahmed Hamid, Diana Aga

Auditorium Room 1

Municipal wastewater, treated and untreated, can provide tremendous information on biomarkers of disease outbreaks, estimate consumption of illicit drugs, and ecosystem exposure to

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hazardous chemicals. Liquid chromatography-mass spectrometry (LC-MS) and gas chromatography-mass spectrometry (GC-MS) have been used in the analysis of pollutants in wastewater, as well as in wastewater-based epidemiology. This workshop will explore the progress and challenges in the detection and identification of trace contaminants, such as pesticides, illicit drugs, pharmaceuticals, personal care products, persistent organic chemicals, endocrine disrupting compounds, and microorganisms in wastewater matrices. The topic will be introduced through data-blitz presentations by early-career scientists, followed by a discussion led by panelists with relevant expertise. The primary goal is to stimulate thoughts and share recent experiences utilizing various instrumental platforms for target and non-target analysis of various types of analytes and their metabolites in wastewater matrices, as well as in activated sludge from wastewater treatment plants. Additional points of discussion are likely to include the use of portable mass spectrometers, applications of ion mobility MS, development of libraries for contaminants, advances in sample preparation, and identification of transformation products resulting from wastewater treatment processes.

06 Forensic Mass Spectral Technology: The Transition from Research to Practical Application (Interest Group: Forensics & Homeland Security)

Presiding: Brittany Casey, Ruth Smith

Auditorium Room 2

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.

07 Data Independent Acquisition Goes Mainstream? (Interest Group: Data Independent Acquisition)

Presiding: Lindsay Pino, Florian Meier

Ballroom A

High levels of reproducibility and data completeness are key features that attract (prote)omics researchers to data independent acquisition (DIA) as they strive towards scaling workflows to hundreds or thousands of samples, derived from single cells or large clinical cohorts.

Taking full advantage of the intrinsically parallel nature of DIA acquisition schemes, advances in bioinformatics and the latest generation of liquid chromatography - mass spectrometry systems, have led to the development of increasingly rapid acquisitions of just a few minutes per sample without compromising proteome coverage. Another notable trend in recent years has been the implementation of ion mobility techniques to add an additional dimension of separation and reduce spectral complexity. One striking application thereof is the filtering of interfering background ions for the analysis of very low sample amounts. As DIA traces fragment ions across a peptide's full chromatographic elution time, it also holds great potential for the analysis of post-translational modifications such as phosphorylation, acetylation and ubiquitination. Other areas of active research range from sample multiplexing and spectral library prediction to the exploration of alternative fragmentation methods. This is accompanied by the development of faster, more flexible and user-friendly software solutions.

In this workshop, we invite experts in the field to discuss emerging topics in DIA. The open format will allow beginners as well as advanced DIA researchers to actively participate and bring their own topics to the discussion.

08 Single-cell proteomics: From Sample Preparation to Data Analysis (Independent)

Presiding: Ying Zhu, Ryan Kelly

Ballroom B

There is growing interest in extending LC-MS-based proteomics analysis to single cells. Single-cell proteomics can reveal critical insights on biological systems that are masked in bulk analysis, including diverse cell populations, cell developmental trajectories, and tissue microenvironments. However, because of the orders-of-magnitude reduction in sample input relative to bulk-scale proteomics, the comprehensive characterization of the single-cell proteome is still immature and confronts many technical challenges. These challenges include but are not limited to cell isolation, sample preparation, LC separation, MS measurement, data analysis, and visualization. As such, new technologies are required to advance this field.

We believe these technical challenges can bring exciting research opportunities for the ASMS community. To promote this research field, we will organize a single-cell proteomics workshop in ASMS 2022. The workshop will focus on two major topics: (1) We will invite the leading scientists to provide an update of technology advances and biological applications in the field; (2) We will set up roundtable discussions to discuss and summarize the remaining challenges, further directions, and to answer the questions from attendees.

Invited speakers:

Karl Mechtler, Head of Protein Chemistry Facility, Research Institute of Molecular Pathology (IMP), Vienna, Austria

Jennifer Van Eyk, Professor at Cedars-Sinai Medical Center, Los Angeles, USA

Marvin Thielert, PhD Graduate Student at Max Planck Institute of Biochemistry, Munich, Germany

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09 How to Kick Start Your Career in Industry (Part 2) (Interest Group: Young Mass Spectrometrists)

Presiding: Chris Pulliam, Laura Sanchez

Room 101

The Young Mass Spectrometrists workshop part 2 will focus on a panel discussion where representatives from industry, pharma, sales, and startup companies will discuss aspects of their personal journeys and opportunities that highlight not only how to break into this sector but also challenges and benefits to these positions. 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 will be composed of representatives from industry, pharma, sales, and startup companies career paths to provide a targeted discussion of these types of career opportunities for young researchers who have mass spectrometry skills. Time permitting and level of interest, 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.

10 Cannabis & Hemp Science: The Importance of Mass Spectrometry (Independent)

Presiding: Asra Gilani, Eberhardt Kuhn

Room 102

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. Most recently, certain cannabinoids have been shown to block the Covid-19 virus from entering human cells.

Mass spectrometry played an important role in this ground-breaking discovery. In this session, the author will review their study of "Cannabinoids and Covid" and we will use that work as the centerpiece for reviewing and discussing current and future applications of mass spectrometry in advancing cannabis/hemp science.

GOALS:
Deliver key opinion leader panel discussions on novel applications of cannabis and hemp in the medical arena as well as future directions.
Foster discussions regarding the applications of mass spectrometry to cannabis and hemp science and research.
Encourage expanded use of mass spectrometry in cannabis/hemp applications by sharing information and discussing emerging growth areas.

PANELISTS

- Richard van Breemen (Oregon State University)
- Jack Henion (Advion, Cornell University)
- Matt Vergne (Lipscomb University)

11 Characterizing Greatness: Celebrating Fred McLafferty (Independent)

Presiding: Mariam ElNaggar, Joseph Loo

Room 103

This workshop will offer participants the opportunity to participate in sharing knowledge, experiences, and skills developed from working (directly or indirectly) with Fred McLafferty. Our panel will include mass spectrometrists with different perspectives, toward understanding the fullness of Fred's career and honoring what made him an inspiring and influential mentor, collaborator, and scientist.

Sharing anecdotes and lessons learned will be encouraged and stories compiled, taking a look at different types of interactions (e.g., former undergraduate and graduate students, postdoctoral scientists, professional nemeses, etc.); different areas of lesson application (e.g., academic, industrial, and other fields); and different areas of expertise and interest over time--noting his front end interests in choices of things to analyze and source developments, work inside the instrument in terms of maximizing detection and fragmentation, on the data analysis side of things, and beyond. Panelists and contributors will be encouraged to make quick slides showing the results of their interactions and evolution of their work, but primarily as a backdrop for conversations of what lessons have persisted.

Networking will be encouraged, resulting in also compiling a meta-oral-history and building potential collaborations, as scientists from different areas of interest come together.

12 Democratizing Metabolomics: Lessons learned and future directions from US regional core facilities (Interest Group: Metabolomics)

Presiding: Maryam Goudarzi, Thomas Horvath, Tytus Mak

Room 200 BC

NIH Regional Comprehensive Metabolomics Resource Cores (RCMRCs) are home to highly specialized teams of scientists, state-of-the-art instrumentation, and cutting edge bioinformatic pipelines that are capable of processing and analyzing the most complex problems in the field. RCMRCs are at the forefront of bioanalytical innovation, and have played a pivotal role in the inexorable rise of metabolomics as a critical platform for life science, environmental, and clinical research. As a tribute to their success and to learn from their decade-long expertise as US regional cores, we have invited a representative from each RCMRC to highlight their distinct services on addressing the needs of the metabolomics community. Each RCMRC representative will have a maximum of 5 minutes to provide a synopsis of the capabilities and expertise of their respective cores, followed by a 10 minute overview given by a representative from the NIH Metabolomics Common Fund on current consortium efforts. The workshop will conclude with a guided 30-minute open panel discussion. The list of confirmed representatives include:

- Prof. Timothy Garrett, Co-Director of the Southeast Center for Integrated Metabolomics (SECIM)
- Prof. Rick Higashi, Director of the Resource Center for Stable Isotope-Resolved Metabolomics (RC-SIRM)

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- Prof. Susan Sumner, Director of Eastern Regional Comprehensive Metabolomics Resource Core (ERCMRC)
- Dr. Tong Shen, Manager of West Coast Metabolomics Center at UC Davis (WC3MRC)
- Dr. Maureen Kachman, Managing Director of Michigan Regional Comprehensive Metabolomics Research Core (MRC2)
- Dr. Douglas Sheeley, Program Leader of the NIH Metabolomics Common Fund

We believe that this workshop will be especially informative for the metabolomics research community and will be a great opportunity to examine the utility of the broad experience in these cores to best serve our research needs.

13 Allyship: Embracing Diversity and Inclusion in Your Workplace (Interest Group: Career Development)

Presiding: Lucinda Hittle, Troy Wood

Room 200 DE

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 hear from a panel discussion of allyship, including 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.

14 Cloud Resources for Proteomics Analysis (Independent)

Presiding: Pratik Jagtap, Timothy Griffin, Magnus Palmblad

Room 200 FG

The Proteome Informatics Group (iPRG) from ABRF is planning a series of online tutorials in the Summer/Fall of 2022. These online tutorials would introduce mass spectrometry-based proteomics researchers to cloud computing resources. This will include workflows based on Nextflow, the TransProteomic Pipeline (TPP), and Galaxy Resources.
In this evening's workshop, speakers will offer a glimpse of what would be covered at the workshop and will have a discussion regarding cloud-computing resources available to researchers.

The online workshops will provide video tutorials that researchers can access and follow along at their own pace. No prior experience with cloud computing is assumed. Registrants will be introduced to the dataset and cloud computing in general, followed by detailed tutorials for each cloud-computing platform, where participants will be able to follow the systematic instructions for each cloud-based workflow.

TENTATIVE SCHEDULE:
Introduction (Timothy Griffin): 5 minutes

Talk 1: TPP resources for Proteomics Analysis (Michael Hoopmann): 10 minutes

Talk 2: Galaxy resources for Proteomics Analysis (Pratik Jagtap): 10 minutes

Talk 3: Nextflow for Proteomics Analysis. (Veit Schwämmle): 10 minutes

Talk 4: Use of Nextflow resources for Long Read Proteogenomics (Gloria Sheynkman): 10 minutes

Panel discussion wherein speakers will answer questions from attendees. 30 minutes.

15 Ion Mobility Spectrometry: What's next? (Interest Group: Ion Mobility MS)

Presiding: Kelly Hines, Xueyun Zheng,

Room 200 HI

Over the last decade, there have been significant advancements in the technology development of ion mobility spectrometry (IMS). Commercial IMS platforms with high resolution separation capabilities are now available from several different vendors. Today's instrumentation is more flexible than previous iterations by allowing the user to control resolving power, by adjusting the length or time of the separation, to suit the needs of the experiment. In this workshop, we will take a look to the future of IMS to explore potential new applications unlocked by today's IMS instruments, as well as new ion mobility technologies that are being developed. Lastly, we will open the session for discussion on the directions and challenges that IMS users envision will emerge in the next decade.

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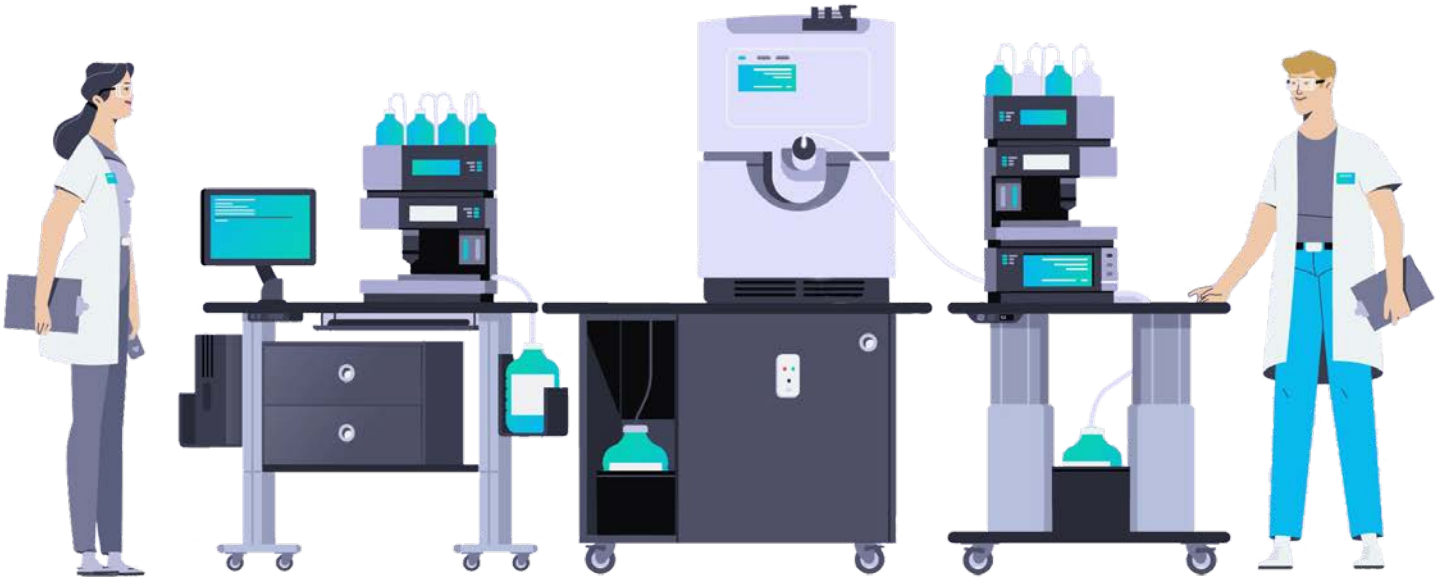

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