

73rd ASMS Conference on Mass Spectrometry & Allied Topics, June 1 – 5, 2025
TUESDAY NETWORKING SESSION & EVENING WORKSHOPS

TUESDAY NETWORKING SESSION, 12:00 - 1:00 pm

Networking Session: Hispanics and Latinx in MS

Presiders: Adriana Zardini Buzatto, Rafael Montenegro Burke
Poster-Exhibit Hall, 12:00-1:00 pm

This networking session will act as the official Hispanics and Latinx in MS Special Interest Group meeting at the ASMS Conference. Last year in Anaheim, we held the second Hispanics and Latinx in MS meeting at ASMS (networking session), which was highly successful with over 70 attendees and strong engagement. During the networking session, we gave all candidates for our Executive Committee a chance to introduce themselves and why they were interested in serving the group. Additionally, we had short talks with members selected for an oral session. The elected leadership group, advised by the founders, is planning the next steps for the group, which includes the ASMS networking session. At this networking session, we will plan activities to allow for social, professional, and research exchanges and interactions. We will highlight our younger member's research by keeping the opportunity to present a short talk (we will solicit abstracts for selection). We feel this is important, as it is quite difficult to get a talk at the ASMS Conference, and this could give our younger members a boost in confidence to speak at a national meeting. Additionally, we will hold a career advisement session. Lastly, we would like to hold soft gathering Network Sessions to allow for more informal chats and research/professional advice meeting time.

TUESDAY EVENING WORKSHOPS, 5:45 - 7:00 pm

01 De Novo Peptide Sequencing: Ready For Prime Time?

Independent

Presiders: Justin Sanders, Wout Bittremieux, William Fondrie
Room 307-308

In recent years, deep learning-based de novo peptide sequencing has made significant advances, demonstrating remarkable performance in interpreting mass spectrometry data. Despite these successes, researchers still face numerous questions when applying these tools in practice. This workshop aims to demystify deep learning-based de novo sequencing, providing attendees with a clear understanding of the state of the field, best practices, and practical insights through interactive discussions and live demonstrations.

With a growing number of de novo tools and approaches available, researchers often find themselves asking:

- Which de novo tool should I use? With so many options available, selecting the right one can be challenging. We will present insights from a community-driven benchmarking effort comparing over a dozen de novo tools.
- What are the best practices for de novo sequencing? We will explore common pitfalls, practical considerations, and specific use cases, including immunopeptidomics and metaproteomics.
- How can I ensure confidence in my results? Unlike sequence database searches, de novo sequencing lacks well-established false discovery rate control methods. We will discuss best practices for assessing confidence and data quality.
- Can de novo sequencing solve my specific problem? We invite attendees to bring their own data and explore the power of de novo sequencing in real time. Through live analysis, we aim to uncover unexpected insights together.

Join us for an engaging session where we cut through the complexity and uncover the potential of deep learning-driven de novo peptide sequencing in mass spectrometry research!

02 Art, Museums and Archaeology

Art, Museums and Archaeology Interest Group

Presiders: Alba Alvarez Martin, Paul Haynes
Room 309-310

The study of archaeological specimens, artworks, and other cultural heritage objects by mass spectrometry requires the adaptation of techniques developed for biomedicine, forensics, or industrial and natural product research, to diverse fields such as anthropology, paleontology, archaeology, natural history, and art history. This introduces unique issues and challenges and often requires some creative problem-solving. Sharing information on some of the more unusual samples analyzed and projects undertaken is helpful for all fellows professionals in the fields, and it will be a unique and inspiring opportunity for other colleagues working on different topics.

This workshop will feature lightning talks selected from ASMS poster abstracts - students and fellows are encouraged to volunteer in advance by contacting the organizers.

Lightning talks will be followed by audience Q&A with a panel of academic, government, public museums and private institution scientists to discuss areas of interest in the field.

Topics may include such things as: ethics and permissions involved in analyzing culturally sensitive samples; considerations for historical and contemporary sample contamination; the risk of damage to objects as a result of analysis; the implementation of new minimal invasive sampling techniques; discerning the importance of chemicals identified from an analyte removed from context; sample-limited preparation and recovery approaches for rare and precious analytes; the significance of preservation and prediction of material degradation; the importance of a maintaining fluid communication with conservators and curators; employment, funding, and fellowship opportunities in the field; and much more.

03 Spectral Library Basics - What is an Identification?

Mass Spectral Libraries Interest Group
Presiders: Tim Stratton, Douglas Slotta
Room 314-317

What information is available to provide for an identification? What is the value that should be placed on different pieces of information? How much information is required to provide a confident identification? What is the level of confidence that is required for a specific need? We will discuss viewpoints and potential answers around all of these questions through a series of presentations across a wide range of applications. Afterwards, we will hold a panel discussion between the experts and members of the audience. In addition, we will continue our interactive survey that we conduct every year.

04 Native MS: Strategies for Advancing Protein Characterization in Industry and Academia

Native Mass Spectrometry Interest Group
Presiders: Kristine Parson, Carter Lantz
Ballroom II

Native mass spectrometry (nMS) is a transformative analytical technique crucial for analyzing biomolecules, particularly proteins and protein complexes, while preserving their native conformations and non-covalent interactions under near-physiological conditions. This allows researchers to interrogate the structure, dynamics, and interactions with other biomolecules and compounds as they exist naturally. As a result, nMS has been able to provide valuable insights into complex biological processes like protein folding, ligand binding, and protein assembly formation. It is also instrumental in drug discovery and development, as it can provide relevant information on interactions between therapeutic compounds and targets including the specificity and efficacy of those interactions. The technique's capability to provide detailed molecular data enhances research rapidly and accurately in biochemistry, molecular biology, and pharmacology, confirming its indispensable role in life sciences.

This workshop will highlight recent advancements in nMS technology, focusing on how these innovations are applied across diverse research areas and how they are being used to solve complex problems. The workshop is designed to be informal and welcoming, serving as a valuable resource for both newcomers and those well-versed in nMS to ask questions and find inspiration for their own research.

Effectively using nMS requires technical expertise so the instrument can be optimized for the biological systems being studied. Traditionally, the workshop facilitates collaboration and knowledge exchange between academia and industry by featuring a diverse group of experts who provide brief presentations. The presentations, along with an open discussion led by the organizers, aim to promote productive dialogue among participants.

05 Young Mass Spectrometrist Workshop: Graduate School Through Early Career Forum

Young Mass Spectrometrists Interest Group
Presiders: John Stutzman, Jeremy Manheim
Ballroom I

The Young Mass Spectrometrist (YMS) Workshop has historically been an open forum for graduate students, post-docs, and early career scientists to question and receive career feedback from a diverse panel. A highlight of this workshop is the ability to ask direct questions and receive candid feedback, which has been a key piece of positive feedback from attendees. The YMS workshop at the 2025 ASMS conference will continue this practice with some minor changes based on attendee feedback from 2024. The two chairs (Jeremy Manheim and John Stutzman) will begin by gathering a diverse panel with considerations of career type (academia, government, industry) and position (technical support, researcher, project leader, hiring manager) as well as background (gender, race, culture). At the beginning of the workshop, approximately 15 minutes will be allocated for the panel to communicate a short introduction to the attendees. Once completed, the chairs will start questions from the attendees (approximately 60 minutes). 2024 feedback indicated that attendees wanted more time for Q&A, so condensing introductions and opening comments will ensure increased interaction. Attendees' questions may be asked directly through microphone or a question box. The chairs will have several preprepared topics and questions to help spark/facilitate discussion if the dialogue begins to slow. Preprepared topics will cover the spectrum of graduate school, post-doctoral positions, finding jobs, and early career topics. 2024 feedback also indicated a focus on graduate school and students, so there will be efforts to be inclusive over all early career mass spectrometrists.

06 Unlocking the Full Potential of Discovery and Early Development DMPK Support: Revolutionizing Efficiency, Innovation, and Integration with Mass Spectrometry

DMPK Interest Group
Presiders: HsinPin Ho, Yongle Pang
Ballroom III

In the pharmaceutical industry, bioanalytical outsourcing is common. However, companies may also maintain various portion of DMPK studies. This workshop delves into the scientific and operational aspects of supporting DMPK early discovery and preclinical stages, ensuring superior efficiency, cost-effectiveness, and data integrity.

Presenters will discuss strategic methodologies and innovative practices that enable companies to excel in DMPK and early development support. In addition, other insights for GXP support will be leveraged, allowing lab practices to adapt to new challenging technologies, focusing on risk-based approaches and prioritizing sustainability to ensure necessary compliance while technology advancements.

Attendees will gain a comprehensive understanding of DMPK support in the pharmaceutical industry, including embracing innovation, controlling data integrity with digital technologies, achieving expedited turnaround times, and maintaining seamless real-time knowledge exchange and proficient troubleshooting capabilities. The workshop will feature interactive discussions on strategies and practices that help

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pharmaceutical DMPK support, achieving unparalleled bioanalytical capabilities and driving scientific advancements.

TUESDAY EVENING WORKSHOPS, 5:45 - 7:00 pm

08 FTMS Community Resources: Access, Education, and Data Analysis

FTMS Interest Group

Presiders: Yury Tsybin, Martha Chacon-Patino

Room 336

Fourier transform mass spectrometry (FTMS), including FT-ICR, Orbitrap, and Charge Detection MS (CDMS), is a cornerstone of modern mass spectrometry, offering unparalleled resolution and accuracy. However, both newcomers and experts face challenges - newcomers in grasping fundamental principles and experts in staying updated with evolving methodologies, instrumentation access, and data analysis solutions.

The 2025 workshop aims to strengthen the FTMS community by fostering collaboration, sharing resources, and addressing key areas of interest. It will provide a platform to exchange insights, refine methodologies, and contribute to the development of next-generation FTMS applications.

Key Focus Areas:

1. **Access to FTMS Instruments:** We will explore global availability and accessibility, covering open-access FTMS facilities, project initiation at leading institutions, and international FTMS networks. The goal is to expand access and promote collaborative research.
2. **Teaching FTMS Principles:** We will focus on developing and sharing educational materials, including animations and tutorials, to enhance FTMS teaching at all levels. We aim to build a centralized repository of resources to support educators and learners.
3. **Data Analysis Challenges & Solutions:** Addressing the complexities of FTMS data processing, we will review available tools, discuss innovations, and identify gaps in existing workflows. The goal is to develop and share improved analytical pipelines.

Workshop Outcome:

Participants will collaborate on creating a centralized web-based resource featuring:

- A catalog of accessible FTMS instruments.
- Standardized educational materials.
- A repository of data analysis tools and best practices.

This initiative will strengthen the FTMS community, promoting engagement, education, and innovation in FTMS research and applications.

09 Process Considerations for Current Nucleic Acid Therapeutics and Emerging Modalities

Oligonucleotides and Nucleic Acids Interest Group

Presiders: Varun Gadkari, Keeley Murphy, Robert Schuster

Room 339-340

This workshop proposal is submitted by Prof. Varun Gadkari (University of Minnesota), Keeley Murphy (Thermo Fisher Scientific), and Dr. Robert Schuster (GSK) for a workshop hosted by the ASMS Oligonucleotides and Nucleic Acids Interest Group.

Nucleic acids continue to be at the forefront of biomedical research across industry and academia. The annual ASMS workshop session allows the community to gather interested researchers in this space to exchange knowledge and ideas.

This year, we will focus on the ever-challenging process development landscape within the nucleic acid therapeutic space.

As the investment in nucleic acid therapeutic research continues to increase, new challenges are emerging within process development and quality assurance, requiring unique analytical solutions that are often highly amenable with mass spectrometry. The resulting resurgence of interest in nucleic acid mass spectrometry and its applications in the pharmaceutical industry are being met with new process requirements, presenting new challenges for design and implementation. Furthermore, nucleic acid-based therapeutics themselves are rapidly evolving with new "next-generation" modalities emerging within this subfield. In this workshop we will host a panel of researchers from academia and industry to provide insight into the continuously evolving landscape of nucleic acid therapeutic product development. The discussion topics will focus on new process challenges, current best practices, and potential regulatory considerations when developing mass spectrometry-based processes for both "traditional" nucleic acid therapeutics as well as emerging next-generation modalities. The aim is to include 4-6 panelists who will have ~7-10 minutes each to introduce themselves, outline their background and area of expertise, and provide a brief viewpoint on current therapeutic development challenges, mitigation strategies, and process considerations. The introductions will be followed by an open-planned discussion with the audience.

10 Fundamentals of Electrospray Ionization

Fundamentals Interest Group

Presiders: Rachel Loo, Cajetan Neubauer

Room 341-342

A generation after soft-ionization techniques have revolutionized mass spectrometry, advances in our ability to control the ionization of biological samples remain a critical challenge. In many experiments, the ionization process still fundamentally limits the scope and utility of the downstream mass spectrometric analyses.

The 2025 evening workshop will therefore revisit the physical chemical mechanisms of electrospray ionization (ESI), exploring both current knowledge and open questions: What are the known and unknown aspects of ESI mechanisms? How can a deeper understanding of ESI improve data quality in metabolomics, proteomics, and single-cell studies? What approaches are currently being explored to overcome the many limitations and artifacts of ESI? What are the major practical and theoretical challenges in ESI today? Could future approaches enable single-molecule sensitivity in mass spectrometry?

Presenters: Rachel Loo (UCLA), Lars Konermann (Western University, Canada), Anyin Li (University of New Hampshire), Derek Stein (Brown University), Alexander Makarov (Thermo Fisher Scientific). Short presentations are followed by an open forum panel discussion. Please feel free to email questions or other contributions for the discussion also in advance (rloo@mednet.ucla.edu and caj.neubauer@colorado.edu).

11 Plastics, Polymers and Replacement Chemicals Part 1: Recycling, Deconstruction, and Redesign of Polymeric Materials

Energy & Biofuels, Exposomics, and Polymeric Materials Interest Groups

Presiders: Anthony Gies, David Stranz, Christopher Ruger
Room 343-344

This is part one of two-part workshop: (1) Polymers and Energy & Fuels interest groups will present the 1st workshop focusing on aspects of polymer/plastics recycling and (2) the Exposomics interest group will delve into the exposure aspects of these materials. The overall goal is to highlight the role of mass spectrometry in addressing complex challenges and growing environmental concerns over the waste streams of polymeric materials at the end of their life cycles, and how they can be reintroduced into new life cycles. In this first part, we will discuss strategies for recycling, upcycling, and redesign of polymeric materials. We will evaluate the role of advanced mass spectrometry techniques to enable this research area in the development of renewable materials.

This participatory workshop includes a series of short tutorial lectures. The lead talking points with the audience will include;

- What type of polymers/plastics can be reused and what are the current obstacles?
- Upcycling processes, including chemical and biological deconstruction of polymers
- Use of deconstructed products and analytical opportunities, including investigation of deconstruction chemistry and mechanisms to further this research.
- Circular polymer processes, such as replacement of petrochemically-derived feedstocks. Opportunities in application of advanced mass spectrometry to investigate reaction and degradation mechanisms to aid redesign of monomers for circular polymers.

Discussion panel will be composed of experts from variety of disciplines. They will be tasked with initiating discussions on challenges and potential solutions that mass spectrometry can offer in this economically impactful research area.

12 Proteomics Data Analysis: From Identification to Quantification

Bioinformatics MS Interest Group
Presiders: Fengchao Yu, Daniel Polasky
Room 345-346

This workshop aims to provide an overview of proteomics data analysis for anyone interested in proteomics, from novice to expert. The workshop will feature a brief overview of general principles of DDA and DIA data analysis, followed by a panel discussion of emerging trends and ongoing challenges. Participants will gain insights into key principles of peptide identification and quantification, exploring widely used computational tools and their applications in real-world research.

The session will begin with a brief overview of peptide identification and quantification for DDA and DIA data, covering the fundamental principles and introducing popular tools such as MaxQuant, DIA-NN, and MSFragger incorporated with FragPipe. Participants will learn how these tools process mass spectrometry data to accurately identify peptides and proteins, as well as the many approaches to quantitation and their key

pros and cons. Emerging trends in the field, such as the role of machine learning and AI, will also be highlighted to seed discussion topics for the panel to follow. A second presentation on specialized applications of proteomics data analysis, including HLA peptidome and glycoproteomics research, will highlight key challenges in field that will serve as starting points for the panel discussion.

The panel discussion will aim to offer commentary on the current state of the field and provide interactive discussions with participants to enhance their understanding of advanced proteomics methodologies and gain practical knowledge to apply these techniques in their own studies.

13 Lab Management Software: Necessity or Luxury?

Analytical Lab Managers Interest Group
Presiders: Maryam Goudarzi, Caroline Chidley
Room 347-348

While lab management software is not a necessity for all labs, there has been an increase in demand for such software in service facilities across different sectors. The decision to invest in such software tools and which tool in specific is entirely dependent on each individual lab's operations, complexity of the offered services, staff and budget among other factors.

In this workshop we will discuss:

1. Popular commercial software solutions
2. Their pros and cons based on attendees' experiences
3. Points to consider when investing in a system, including key features
4. Staff training
5. Adoption and data migration

We will invite an open discussion with our attendees about their expectations from the software on:

1. Improved efficiency: Lab management software can automate many tasks, such as sample tracking, data entry, and report generation.
2. Reduced errors: Lab management software can help reduce errors by standardizing processes and
3. Increased compliance, including meeting regulatory requirements (i.e. FDA and HIPAA).
4. Improved Data management: Lab management software can help labs store and manage their data more effectively. This can make it easier to find, analyze data and collaborate on projects.

We will also discuss factors that lead to hesitation in adopting such systems in various labs, including software features, budget and getting buy-in from the staff.