2025 Advancing Mass Spectrometry for Biophysics and Structural Biology

Georgia Institute of Technology | Atlanta, GA USA

~ AGENDA ~

Sunday, July 20, 2025

Venue: Marcus Nanotechnology Building (unless otherwise indicated)

PANEL DISCUSSION

3:00-5:00 p.m. "Affordable Native Mass Spec Solutions: Community and Vendor Conversation"
Panelists:

- Weijing Liu – Vertical Marketing Manager, Thermo Fisher Scientific
- Roy Martin – Senior Manager, Waters
- Paul Speir – Senior Vice President, Commercial Operations, Bruker
- Shane Tichy – Associate Vice President LC/MS R&D, Agilent

CHECK IN

Marcus Nanotechnology Building, Atrium 4:30-7:00 p.m.

CONFERENCE OPENS

Session Chair: Vicki Wysocki, Georgia Institute of Technology

6:30 p.m. *Welcome Refreshments*

7:00 p.m. Welcome Remarks

Opening Plenary Lecture - Stephan Rauschenbach, University of Oxford - "Atomic Resolution Molecular Imaging by Scanning Probe and Electron Microscopy Based on Soft-landing Electrospray Ion Beam Deposition"

7:45 p.m. Andrew McShan, Georgia Institute of Technology - "The Power and Pitfalls of AlphaFold for Structure Prediction Beyond Rigid Globular Proteins"

8:10 p.m. Discussion

8:30 p.m. *Reception*

10:00 p.m. Adjourn

Monday, July 21, 2025

Venue: Marcus Nanotechnology Building (unless otherwise indicated)

8:00 a.m. Breakfast

MONDAY A.M. SESSION 1: NEW METHODS I

Session Chair: Richard Vachet, University of Massachusetts Amherst

9:00 a.m. Charlotte Uetrecht, Centre for Structural Systems Biology, Deutsches Elektronen-Synchrotron, University of Lübeck - "Flying Viruses – Mass Spectrometry Meets X-rays"

9:30 a.m. Joshua S. Sharp, University of Mississippi - "Radical Footprinting in Mammalian Whole Blood of a Murine Diabetes Model"

10:00 a.m. **Hot Topic Talk 1:** Peter Armentrout, University of Utah - "Influence of Methylating the Serine Side-chain on the Decomposition of Protonated Asparaginyl Serine using GIBMS, IRMPD, and Theoretical Modeling"

10:15 a.m. Discussion

10:30 a.m. *Coffee Break*

MONDAY A.M. SESSION 2: NATIVE MASS SPECTROMETRY I

Session Chair: Mary T. Rodgers, Wayne State University

11:00 a.m. David Russell, Texas A&M University - "Influences of Buffers and Water on Protein Structures, Stabilities, and Dynamics: A Variable Temperature-native ESI MS Perspective"

11:30 a.m. Ying Ge, University of Wisconsin - "Advancing Native Top-down Proteomics for Structural and Proteoform Analysis"

12:00 p.m. Discussion

12:15 p.m. *Lunch*

MONDAY P.M. SESSION 1: ADVANCES in INSTRUMENTATION I

Session Chair: Si Wu, University of Alabama

1:30 p.m. Jakub Ujma, Waters Corporation - "The Design and Characterisation of a New Charge Detection Mass Spectrometry (CDMS) Instrument for the Analysis of Megadalton-Sized Molecules"

2:00 p.m. Abraham Badu-Tawiah, Ohio State University - "Dynamic Spray Mass Spectrometry"

2:30 p.m. **Hot Topic Talk 2:** Tarick El-Baba, Kavli Institute for Nanoscience Discovery - "Native and Top-down Mass Spectrometry Reveals Remodeling of Brain-derived mGluRs in Major Depressive Disorder"

2:45 p.m. Discussion

3:00 p.m. *Coffee Break*

MONDAY P.M. SESSION 2: IMAGING and EMERGING CHALLENGES

Session Chair: Nicholas Borotto, University of Nevada

3:30 p.m. Facundo Fernández, Georgia Institute of Technology - "A Mass Spectrometry Imaging Annotation Workflow Combining Cyclic Ion Mobility and Machine Learning Molecular Predictions"

4:00 p.m. Amanda Hummon, The Ohio State University - "Mass Spectrometry Imaging and Proteomic Analysis of Liposomes in 3D Cell Cultures"

4:30 p.m. **Hot Topic Talk 3:** Varun Gadkari, University of Minnesota - "Antibodies to mRNAs: Addressing Emerging Challenges in Biotherapeutic Characterization by Expanding the Native Mass Spectrometry Toolkit"

4:45 p.m. Discussion

5:00 p.m. *Break (on your own)*

6:00 p.m. *Dinner*

MONDAY EVENING SESSION: GLYCO & CARBOHYDRATES + FLASH TALKS I

Session Chair: Ronghu Wu, Georgia Institute of Technology

7:00 p.m. John Klassen, University of Alberta - "Deciphering the GlycoCode through Native Mass Spectrometry"

7:30 p.m. Gabe Nagy, University of Utah - "Integrating Cyclic Ion Mobility Separations, Tandem Mass Spectrometry, and Collision Cross Section Measurements for Carbohydrate Sequencing"

8:00 p.m. **Poster Flash Talks – Session I**

Raihana Afroz, University of Minnesota - “Native Charge Detection Mass Spectrometry Measurements of Messenger RNA”

Ryan Allen, Georgia Institute of Technology - “Sometimes All You Need is a Little HeLP: Heme Labeling by Proximity Unveils Heme Regulation of the Insulin Receptor”

Edvaldo Maciel, Technical University of Darmstadt - “Flow-induced Dispersion Analysis – Mass Spectrometry (FIDA-MS) for Structural Characterization of Native Proteins from Conventional Molecular Biology Buffers”

Aleksandr Melikov, University of Geneva - “G-quadruplex – Ligand Interaction Biophysics Explored by Native Mass Spectrometry and Trapped Ion Mobility Spectrometry”

Noor Naseeb, University of Oxford - “Investigation into the Dynamic Structure of Heat Shock Proteins using Electrospray Ion Beam Deposition and Cryo-electron Microscopy”

Robert Rider, Texas A&M University - “Quantitation of Heterogenous Protein Samples Utilizing Orbitrap Charge Detection Mass Spectrometry”

Nirmal Saha, Georgia Tech - “Unlocking Nature’s Chemical Diversity: Genome Mining Strategies for Peptide Halogenases and Their Catalytic Potential”

John Yates, Scripps Research Institute - “Determining the Structural Consequences of the Specific Distribution of N-glycans on Candidate Vaccines against HIV”

8:30 p.m. **Poster Session I** (Odd #’s) and Reception

10:00 p.m. Adjourn

Tuesday, July 22, 2025

Venue: Marcus Nanotechnology Building (unless otherwise indicated)

8:00 a.m. *Breakfast*

TUESDAY A.M. SESSION 1: ION MOBILITY

Session Chair: Matt Bush, University of Washington

9:00 a.m. Christopher Chouinard, Clemson University - "High-resolution Ion Mobility-mass Spectrometry: Uncovering New Structural Details for Drug Compounds"

9:30 a.m. Rebecca Beveridge, University of Strathclyde - "IM-MS Unveils Global Protein Conformations in Response to Conditions that Promote and Reverse Liquid–liquid Phase Separation"

10:00 a.m. **Hot Topic Talk 4:** Michael Armbruster, University of Michigan - "Enhanced Detection of Targeted Phospholipids by Native Ion Mobility–mass Spectrometry with Selective Lipid Binding and Collisional Ligand Ejection"

10:15 a.m. Discussion

10:30 a.m. *Coffee Break*

TUESDAY A.M. SESSION 2: STRUCTURAL PROTEOMICS I

Session Chair: Ian Webb, Indiana University Indianapolis

11:00 a.m. David Schriemer, University of Calgary - “Redesigning the Crosslinking Reaction for High-fidelity Cellular Interactomics: Almost There”

11:30 a.m. *~ Remote Presentation ~* Andrea Sinz, Martin-Luther-University Halle-Wittenberg - "Structural Characterization of ‘Difficult’ Proteins by Cross-linking Mass Spectrometry using MS-cleavable Cross-linkers"

12:00 p.m. *Lunch*

TUESDAY P.M. SESSION: PHARMA / CLINICAL I

Session Chair: Rakesh Singh, Georgia Institute of Technology

1:15 p.m. Blaine Roberts, Emory University (Agilent Sponsored Speaker) - "Structural Characterization of Proteins Involved in Neurodegenerative Disease Using Ion Mobility and Electron Capture Dissociation"

1:45 p.m. Jon Williams, AbbVie - "Evolving Mass Spectrometry to Enable its Application in Structural Biology and Biophysics Activities within Small Molecule Drug Discovery"

2:15 p.m. Discussion

2:30 p.m. **AFTERNOON OFF / FREE TIME / Dinner on Your Own**
Georgia Aquarium – For Attendees with Pre-Reserved Tickets Only *(no on-site admissions available)*

TUESDAY EVENING SESSION: NATIVE MASS SPECTROMETRY I

6:45 p.m. *Light refreshments*

Session Chair: Liangliang Sun, Michigan State University

7:00 p.m. Scott McLuckey, Purdue University - "Ion/Ion Reactions in Native Mass Spectrometry: Methods and Instrumentation"

7:30 p.m. Jennifer Brodbelt, University of Texas at Austin - "Probing Protein Interactions using Ultraviolet Photodissociation and Native Mass Spectrometry"

8:00 p.m. **Poster Flash Talks – Session II**

Alexander Deans-Rowe, Georgia Institute of Technology - "A Metabolomics/Proteomics-inspired Workflow to Probe Prebiotic Chemical Systems"

Laura Finazzi, Radboud University - "Steroidal Hormones Fragmentation Mechanisms Revealed by Infrared Ion Spectroscopy"

Weijing Liu, Thermo Fisher Scientific - "High-throughput Molecular Glue Screening via Native Mass Spectrometry and Cryo-EM Analysis"

Fanny Caroline Liu, Florida State University - "Unraveling Multispecific Antibody–antigen Interactions using Tandem-trapped Ion Mobility Spectrometry (Tandem-TIMS)"

Lester Manly, Emory University - "Investigating the Effects of Cu/Zn Loss on Superoxide Dismutase 1 Structure using Ion Mobility and Electron Capture Dissociation"

Jalah Morris, University of California, San Diego - "Advancing Health Disparities Research Through Protein Footprinting on PBMCs"

Lucas Narisawa, University of Washington - "Photo-crosslinking for Identifying Residue-level Interactions Involving Proteins with Intrinsic Disorder"

Daniel Saeedi, Georgia Institute of Technology - "AstroAgents: A Multi-agent AI for Hypothesis Generation from Mass Spectrometry Data"

8:30 p.m. **Poster Session II** (Even #'s) and Reception

10:00 p.m. Adjourn

Wednesday, July 23, 2025

Venue: Marcus Nanotechnology Building (unless otherwise indicated)

8:00 a.m. Breakfast

WEDNESDAY A.M. SESSION 1: NEW METHODS II

Session Chair: Jared Shaw, University of Nebraska-Lincoln

9:00 a.m. Dmitris Papanastasiou, Bruker - "Advances in Hardware Design and Function of the New timsOmni MS Platform"

9:30 a.m. Christian Bleiholder, Florida State University - "UV Photofragments of Native-like Proteins Maintain a 'Memory' of the Precursor Protein Structure"

10:00 a.m. **Hot Topic Talk 5:** Ashlyn Dollar, Indiana University Indianapolis - "Osmolyte-induced Structural Changes in Wild Type and Phosphorylated Alpha Synuclein"

10:15 a.m. Discussion

10:30 a.m. *Coffee Break*

WEDNESDAY A.M. SESSION 2: PHARMA / CLINICAL II

Session Chair: Aneika Leney, University of Birmingham

11:00 a.m. Sara Carillo, National Institute for Bioprocessing Research and Training (NIBRT) - "Tackling Biosimilarity Assessment using Top-down and Middle-down Mass Spectrometry"

11:30 a.m. Ashok R. Dongre, Bristol-Myers Squibb - "Proteomics at Scale - Empowering Biopharmaceutical Discovery & Translational Research"

12:00 p.m. Discussion

12:15 p.m. Lunch - ***Note Different Location:*** *Petit Biotechnology Building (IBB)*
📍 315 Ferst Drive NW – directly across Atlantic Drive, next door

WEDNESDAY P.M. SESSION 1: STRUCTURAL AND NATIVE MS

Session Chair: Elizabeth Duselis, Georgia Institute of Technology

1:30 p.m. Argyris Politis, University of Manchester - "The Functional Dynamics of Membrane Proteins in Physiological Conditions using HDX-MS"

2:00 p.m. Yuqi Shi, Thermo Fisher Scientific (Sponsored talk) - " Advancing HDX-MS Analysis for Enhanced Sensitivity and Resolution"

2:30 p.m. **Hot Topic Talk 6:** Yuan Gao, Georgia Tech - "Interaction of Substrate and Inhibitors with Salmonella FraB Deglycase, a Drug Target"

2:45 p.m. Discussion

3:00 p.m. *Coffee Break*

WEDNESDAY P.M. SESSION 2: NATIVE MASS SPECTROMETRY II

Session Chair: Stephen Valentine, West Virginia University

3:30 p.m. Nina Morgner, Goethe University Frankfurt - "Light Triggered Time-resolved Ion Mobility Mass Spectrometry Allows Investigation of Conformation and Oligomerization in Cryptochromes"

4:00 p.m. Kallol Gupta, Yale University - "Nanoscale Molecular Cartography of the Cellular Membranes"

4:30 p.m. **Hot Topic Talk 7:** Elyssia Gallagher, Baylor University - "Comparing Native-protein Charging and Structures Associated with Different Modeling Techniques"

4:45 p.m. Discussion

5:00 p.m. *Break (on your own)*

6:00 p.m. *Dinner*

WEDNESDAY EVENING SESSION

Session Chair: Steffen Lindert, University of California Los Angeles - Conference Co-Chair

7:30 p.m. ***Closing Plenary Lecture*** - Valérie Gabelica, University of Geneva - "Novel Insights into Native Ion Mobility from Nucleic Acid Studies"

8:15 p.m. Closing Reception

9:30 p.m. Adjourn

POSTER SESSION DIRECTORIES

SESSION I – ODD #'s – Monday, July 21 – 8:30 p.m.

Poster #	Presenter	Affiliation	Poster Title
1	Raihana Afroz	University of Minnesota	Native Charge Detection Mass Spectrometry Measurements of Messenger RNA
3	Ryan Allen	Georgia Tech	Sometimes All You Need is a Little HeLP: Heme Labeling by Proximity Unveils Heme Regulation of the Insulin Receptor
5	Edvaldo Maciel	Technical University of Darmstadt	Flow-induced Dispersion Analysis – Mass Spectrometry (FIDA-MS) for Structural Characterization of Native Proteins from Conventional Molecular Biology Buffers
7	Aleksandr Melikov	University of Geneva	G-quadruplex – Ligand Interaction Biophysics Explored by Native Mass Spectrometry and Trapped Ion Mobility Spectrometry
9	Noor Naseeb	University of Oxford	Investigation into the Dynamic Structure of Heat Shock Proteins using Electrospray Ion Beam Deposition and Cryo-electron Microscopy
11	Robert Rider	Texas A&M University	Quantitation of Heterogenous Protein Samples Utilizing Orbitrap Charge Detection Mass Spectrometry
13	Nirmal Saha	Georgia Tech	Unlocking Nature's Chemical Diversity: Genome Mining Strategies for Peptide Halogenases and Their Catalytic Potential
15	John Yates	Scripps Research Institute	Determining the Structural Consequences of the Specific Distribution of N-glycans on Candidate Vaccines against HIV
17	Sohag Ahmed	West Virginia University	Studying Protein-ligand Interactions using Novel Ionization Methods and In-droplet Hydrogen Deuterium Exchange
19	Madeline Bannon	Baylor University	Nonspecific Carbohydrate Adduction Increases with Increasing Collisional Cross-section of Globular Proteins during Native-ESI MS
21	Kacy Black	Indiana University Indianapolis	Collision Induced Unfolding Detected by Hydrogen/Deuterium Exchange
23	Emily Burningham	Texas A&M University	Intact Mass HDX-MS and IM-MS Reveal Differences in Protein Dynamics Resulting from Native MS Buffers
25	Olivia Dioli	University of Texas at Austin	Mass Spectrometry Reveals Effects of Sequence Complexity on Structure of α-Synuclein
27	Kacie Evans	Texas A&M University	Evaluating Changes to ADP Binding using HDX and Variable Temperature to Provide Insight into the Hydration of SR1 GroEL
29	Austin Graves	Refeyn	Understanding Biomolecular Behavior with Mass Photometry
31	Jared Hampton	Texas A&M University	Analysis of Heterogeneous Higher-order Transthyretin Oligomers using Direct Mass Technology and Ion Mobility-mass Spectrometry
33	Thomas Hughart	West Virginia University	Vibrational Amplitude of Capillary Vibrating Sharp-Edge Spray Ionization (cVSSI) Emitters Influences Ion Intensity of Nucleic Acid and Protein Systems
35	Carter Lantz	Texas A&M University	Analysis of Conformations and Microstates that Form Protein Free Energy Landscapes: A Mass Spectrometry Perspective
37	Cory Lytle	Bruker	Offline Tandem MSn Workflows on the timsOmni Platform for Deep Sequencing of Intact Proteins and mAbs
39	William Moeller	Georgia Tech	Capillary Zone Electrophoresis Based Native Proteomics of E. coli Cell Lysate
41	Zihao Qi	Georgia Tech	Structure and Solution Dynamics of Yeast RAD52 Homolog Mgm101: Snapshots with DNA Reveal a Full Single-strand Annealing Pathway
43	Nicole Rivera-Fuentes	University of Michigan	Ion Mobility-mass Spectrometry and Collision-induced Unfolding Distinguishes Between Tryptophan and Methionine Oxidation and Reveals its Impact on mAbs' Structure and Stability
45	Isabella Rossetti	University of Massachusetts Amherst	Probing Tau Conformations and Early Aggregates using Native Mass Spectrometry
47	Stewart Ryberg	Baylor University	Molecular Dynamic Simulations of Denatured Proteins in Electrosprayed Droplets with H3O+ and Dynamic Protonation
49	Mana Shafaei	Affinisep USA	Fast and Robust Phosphoproteomics Sample Prep with AttractSPE® Disks C18 Tips for High Phosphopeptide Recovery and Identification
51	Liangliang Sun	Michigan State University	CZE-MS is Reproducible and Robust Enough for Large-scale Native and Denaturing Top-down Proteomics
53	Zhixin Xu	Georgia Tech	Characterization of Human Cytomegalovirus Surface Protein by Native MS and Single Particle Methods
55	Hanhao Zhang	Georgia Tech	Revealing N-Glycans on Antigen-specific Antibodies as Biomarkers for Disease State and Outcome by Sample Sparing Multiplexed MALDI Mass Spectrometry Imaging
57	Carter Asef	Andson Biotech	Rapid Online Buffer Exchange with the DynaChip Platform for Complex Biological Analysisg

SESSION II – EVEN #'s – Tuesday, July 22 – 8:30 p.m.

Poster #	Presenter	Affiliation	Poster Title
2	Alexander Deans-Rowe	Georgia Tech	A Metabolomics/Proteomics-inspired Workflow to Probe Prebiotic Chemical Systems.
4	Laura Finazzi	Radboud University	Steroidal Hormones Fragmentation Mechanisms Revealed by Infrared Ion Spectroscopy
6	Weijing Liu	Thermo Fisher Scientific	High-throughput Molecular Glue Screening via Native Mass Spectrometry and Cryo-EM Analysis
8	Fanny Caroline Liu	Florida State University	Unraveling Multispecific Antibody–antigen Interactions using Tandem-trapped Ion Mobility Spectrometry (Tandem-TIMS)
10	Lester Manly	Emory University	Investigating the Effects of Cu/Zn Loss on Superoxide Dismutase 1 Structure using Ion Mobility and Electron Capture Dissociation
12	Jalah Morris	University of California San Diego	Advancing Health Disparities Research Through Protein Footprinting on PBMCs
14	Lucas Narisawa	University of Washington	Photo-crosslinking for Identifying Residue-level Interactions Involving Proteins with Intrinsic Disorder
16	Daniel Saeedi	Georgia Tech	AstroAgents: A Multi-agent AI for Hypothesis Generation from Mass Spectrometry Data
20	Addison Bergman	University of Michigan	Combining Glycan Engineering with Ion Mobility Selected Collision Induced Unfolding (IM-CIU) to Determine Glycoform Influence on Monoclonal Antibody Structural Polydispersity
22	Trisha Brady	University of Massachusetts Amherst	Investigating Conformational Heterogeneity of Various Caspase-9 Maturation States
24	Kymeri Davis	Indiana University Indianapolis	Photocrosslinking of Histones to Study Conformational Changes Induced by Post Translational Modifications
26	Jonathan Eisert	Technical University of Darmstadt	Native Taylor/Non-Taylor Dispersion – Mass Spectrometry (TNT-MS) Allows Rapid Protein Desalting and Ligand Screening using an Unmodified LC-MS Instrument
28	Longping Fu	Georgia Tech	In-depth N-Terminomics Profiling and Dynamics of N-Terminal Proteoforms in Human Cells
30	Ankita Gurav	Indiana University Indianapolis	Structural Analysis of Divalent Cation Bound α-Synuclein by Cross-linking Ion Mobility-Mass Spectrometry.
32	Dustin Huard	Georgia Tech	Elucidating the Connection Between Acid Beta-Glucosidase Variant E326K and Parkinson's Disease
34	Katherine Kenney	Georgia Tech	Progesterone Metabolism and Breast Cancer Risk using Simultaneous Quantitation and Discovery (SQUAD) Liquid Chromatography Mass Spectrometry
36	Aneika Leney	University of Birmingham	A Protein-centric Mass Spectrometry Approach for Species Identification Within Harmful Algal Blooms
38	Rowan Matney	University of Minnesota	Evaluating Stress-induced Stability Changes in Antibody Monomers and Dimers via Collision-induced Unfolding
40	Efe Ozturk	Georgia Tech	Super Resolution Mass Spectrometry Imaging, Multimodal Integration, & Metabolic Barcoding
42	Erika Renbarger	Indiana University Indianapolis	Characterization of Protein Structure using Cleavable Crosslinking and Top-down LC-MS/MS
44	Mary T. Rodgers	Wayne State University	Ammonium Salts Alter the Structures of Protonated 8-Bromo-2¢-deoxyguanosine Populated by Electrospray Ionization versus Those Generated from Acidic Solutions
46	Kejie Rui	University of Georgia	Investigating MSC Immune Suppressive Function with Quantitative Phase Microscopy and Single-cell Spatial Lipidomics
48	John Sentmanat	Georgia Tech	Novel Multi-modal Mass Spectrometry Imaging and Electron Microscopy Instrument to Improve Structural and Chemical Single-cell Visualization
50	Jared Shaw	University of Nebraska-Lincoln	Native MS and Top-down Proteomics Characterization of Ribosome Heterogeneity
52	Xing Xu	Georgia Tech	Glycoproteome and Surfaceome Mapping of Epithelial-to-Mesenchymal Transition Reveals Key Ion Channel Regulation and Novel Biomarkers in Cancer Metastasis
54	Si Wu	University of Alabama	HDX-MS with Integrated Protein Thermal Depletion Reveals Differential Polyclonal Antibody Binding in Two Human AVA Vaccinated Donors
56	Yu Zhou	Centers for Disease Control and Prevention	Assessment of Monoclonal Antibody Structure, Stability, and Developability using Native and Bottom-up LC-MS

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