

Program Schedule

Sunday, July 23rd

Native MS Workshop (optional) 9:30 am-4:00 pm
Welch Hall 2.306

Registration (San Jacinto Conference Center Foyer) 4:30-7:00 pm

Welcome and Keynote Session (San Jacinto Conference Center) 7:00-8:00 pm

Josh Coon, University of Wisconsin 7:00-7:35 pm
Flying & Landing Molecular Elephants

Ruwan Kurulugama, Agilent 7:40-8:00 pm
Protein Structure Analyses using High Resolution Collision Induced Unfolding Enabled by a Modified MOBIE HRIM-QTOF Instrument

Reception (San Jacinto Conference Center) 8:00-9:30 pm

Monday, July 24th

Breakfast (San Jacinto Conference Center) 8:00-9:00 am

Monday Morning Session 1: New Methods I 9:00-10:30 am
San Jacinto Conference Center *Chair: Michael Marty, University of Arizona*

Julia Laskin, Purdue University 9:00-9:25 am
Pushing the Frontiers of Ambient Imaging using Nanospray Desorption Electrospray Ionization Mass Spectrometry

Helen J. Cooper, University of Birmingham 9:30-9:55 am
Latest Developments in Native Ambient Mass Spectrometry

Fanny Liu, Florida State University 10:00-10:25 am
Advancing Top-Down Protein Analysis by Integrated Tandem-TIMS-UVPD-PASEF and Time-Resolved Tandem-TIMS Approaches

Coffee Break (San Jacinto Conference Center) 10:30-11:00 am

Monday Morning Session 2: Advances in Instrumentation I 11:00 am-12:00 pm
San Jacinto Conference Center *Chair: Michael Marty, University of Arizona*

Vicki Wysocki, Ohio State University 11:00-11:25 am
Electrons and/or a Surface: Characterization of Viral Capsids, Glycoproteins, and Nucleoproteins

Robert Schrader, Texas A&M University 11:30-11:55 am
Optimization of a Digital Mass Filter for the Isolation of High m/z Analytes on a Dual Quadrupole-Orbitrap Mass Spectrometer

Lunch (San Jacinto Conference Center) 12:00-1:30 pm

Monday Afternoon 1: Advances in Instrumentation II 1:30-3:00 pm
San Jacinto Conference Center *Chair: Ian Webb, IUPUI*

David Taylor, University of Texas at Austin 1:30-1:55 pm
Combining Mass Spectrometry and Structural Biology to Dissect Novel CRISPR Complexes

Nicholas Borotto, University of Nevada, Reno 2:00-2:25 pm
Collisional Activation of Protein Ions Within a Trapped Ion Mobility Device

Steve Valentine, West Virginia University 2:30-2:55 pm
Enhancing Native Mass Spectrometry with Vibrating Sharp-Edge Spray Ionization

Coffee Break (San Jacinto Conference Center) 3:00-3:30 pm

Monday Afternoon 2: Nucleic Acid Interactions and Proteins 3:30-5:00 pm
San Jacinto Conference Center *Chair: Ian Webb, IUPUI*

Francisco Fernandez-Lima, Florida International University 3:30-3:55 pm
Structural Characterization of DNA-Protein Complexes

Ilya Finkelstein, University of Texas at Austin 4:00-4:25 pm
How can Massively Parallel Studies of Protein-Nucleic Acid Interactions Inform Biochemistry?

Catherine Tremblay, Waters Corporation 4:30-4:55 pm
SELECT SERIES Cyclic IMS and MRT: How HRMS can Aid in Analysis of Intact Proteins and Oligonucleotides

Break (on your own) 5:00-6:00 pm

Dinner (San Jacinto Conference Center) 6:00-7:00 pm

Monday Evening: Hot Topics I 7:15-8:00 pm
San Jacinto Conference Center *Chair: Carter Lantz, Texas A&M University*

Hiruni Jayasekera, University of Arizona 7:15-7:30 pm
Investigating Membrane Protein-Lipid Binding Affinity with Native MS and Mutant Cycles

Virginia James, University of Texas at Austin 7:35-7:50 pm
Investigating Lipid Transporter Protein Interactions using Variable Temperature ESI, UVPD, and Collision Cross Section Analysis

Poster Session I and Reception (San Jacinto Conference Center) 8:00-9:30 pm

Tuesday, July 25th

Breakfast (San Jacinto Conference Center) 8:00-9:00 am

Tuesday Morning Session 1: Beyond Proteomics--Proteoforms 9:00-10:30 am
San Jacinto Conference Center *Chair: Elyssia Gallagher, Baylor University*

Khiry Patterson, Vanderbilt University 9:00-9:25 pm
Establishing Quality Control Procedures for Large Cohort LC-MS/MS Proteomics Studies

Ben Garcia, Washington University-St. Louis 9:30-9:55 pm
Enhanced Understanding of the Chromatin Modification Landscape using Quantitative Mass Spectrometry

Michal Sharon, Weizmann Institute of Science 10:00-10:25 pm
A New Viewpoint on the Treatment of SOD1-Linked Familial ALS

Coffee Break (San Jacinto Conference Center) 10:30-11:00 am

Tuesday Morning 2: Single Ion Methods/Charge Detection 11:00 am-12:00 pm
San Jacinto Conference Center *Chair: Elyssia Gallagher, Baylor University*

Neil Kelleher, Northwestern University 11:00-11:25 am
Label-Free Imaging of Proteoforms in Human Tissues using Individual Ion MS

Martin Jarrold, Indiana University 11:30-11:55 am
Recent Development in Charge Detection Mass Spectrometry

Lunch (San Jacinto Conference Center) 12:00-1:30 pm

Tuesday Afternoon: Computational Strategies 1:30-2:30 pm
San Jacinto Conference Center *Chair: Jim Prell, University of Oregon*

Lars Konermann, University of Western Ontario 1:30-1:55 pm
Peptide and Protein Behavior under ESI Conditions

Steffen Lindert, Ohio State University 2:00-2:25 pm
Computational Protein Structure Prediction from Mass Spectrometry Data

Break/Free time (on your own) 2:30-7:00 pm

Tuesday Evening: Hot Topics II 7:15-8:00 pm
San Jacinto Conference Center *Chair: Daniel Vallejo, Georgia Institute of Technology*

Anna Anders, University of Michigan 7:15-7:30 pm
Ion Mobility and Collision Induced Unfolding Reveal Lipid Nanoparticle-Induced Changes in RNA Structure and Stability

Frederik Lermite, Technical University of Darmstadt 7:35-7:50 pm
Spontaneous electron-based dissociation of native-like cytochrome c oligomers

Poster Session II and Reception

8:00-9:30 pm

San Jacinto Conference Center

Wednesday, July 26th**Breakfast** (San Jacinto Conference Center)

8:00-9:00 am

Wednesday Morning Session 1: New Methods II

9:00-10:30 am

San Jacinto Conference Center

*Chair: Matt Bush, University of Washington*Perdita Barran, University of Manchester

9:00-9:25 am

Translation of *in vacuo* Measurements to Unmet Needs in Medicine and Food SecurityEvan Williams, University of California-Berkeley

9:30-9:55 am

Dynamic Measurements in Charge Detection Mass Spectrometry

Weijing Liu, Thermo Fisher Scientific

10:00-10:25 am

Automated High-throughput online Native MS Screening for Proteins and Protein Complexes Benefiting Cryo-EM Analysis

Coffee Break (San Jacinto Conference Center)

10:30-11:00 am

Wednesday Morning Session 2: Molecular Interactome

11:00 am-12:00 pm

San Jacinto Conference Center

*Chair: Matt Bush, University of Washington*Lan Huang, University of California-Irvine

11:00-11:25 am

Advancing Cross-Linking Mass Spectrometry for Structural Systems Biology

Richard Vachet, University of Massachusetts-Amherst

11:30-11:55 am

Membrane Protein Structure and Binding Interactions in Cells using Covalent Labeling-MS

Lunch (San Jacinto Conference Center)

12:00-1:30 pm

Wednesday Afternoon Session 1: Biotherapeutics and Vaccines

1:30-3:00 pm

San Jacinto Conference Center

*Chair: Rachel Loo, University of California-Los Angeles*Wendy Sandoval, Genentech

1:30-1:55 pm

Direct Analysis of Heterogeneous Biotherapeutics

Brandon Ruotolo, University of Michigan

2:00-2:25 pm

Collision Induced Unfolding of Biotherapeutics: From Proteins to Nucleic Acids and Beyond

Weidong Cui, Amgen

2:30-2:55 pm

Critical Quality Attributes of a Bispecific Antigen-Binding Biotherapeutic – From the Primary Sequence to the Higher-Order Structure

Coffee Break (San Jacinto Conference Center)

3:00-3:30 pm

Wednesday Afternoon Session 2: Structural Proteomics	3:30-5:00 pm
San Jacinto Conference Center	<i>Chair: Rachel Loo, University of California-Los Angeles</i>
<u>Lisa Jones, University of California-San Diego</u>	3:30-3:55 pm
In-Cell Protein Footprinting Coupled to Mass Spectrometry to Study Protein Interactions in Complex Model Systems	
<u>Corrine Lutomski, University of Oxford</u>	4:00-4:25 pm
Native Top-Down for Sequencing G Protein-Coupled Receptors and Related Complexes directly from Native Membranes	
<u>Paul D. Olinares, Rockefeller University</u>	4:30-4:55 pm
Integrating Native MS and Cryo-EM Workflows for Characterization of SARS-CoV-2 Replication Transcription Assemblies	
Break (on your own)	5:00-6:00 pm
Dinner (San Jacinto Conference Center)	6:00-7:20 pm
Plenary Lecture	7:30-8:10 pm
San Jacinto Conference Center	
<u>John Yates, Scripps Research Institute</u>	
Probing the <i>in vivo</i> Structure of Mutant CFTR	
Closing Reception (San Jacinto Conference Center)	8:10-9:30 pm

Monday Posters

1	Afroz, Raihana	U. Minnesota	Evaluation of Repeat Expansion DNA Transcription Inhibitors by Native Mass Spectrometry
2	Armentrout, Peter	U. Utah	Measuring the absolute energy differences between conformers of protonated GlyProGlyGly
3	Bergman, Addison	U. Michigan	An Evaluation of Ion Mobility-Collision Induced Unfolding (IM-CIU) Methods Leveraging Cyclic Ion Mobility Separation for the Evaluation of Protein Dynamics
4	Black, Kacy	IUPUI	Developing various length gaseous electrostatic to covalent crosslinkers: towards understanding the effects of solvation and desolvation on protein structure
5	Bleholder, Christian	Florida State U	Protein (un)folding in the absence of solvent
6	Bush, Matt	U. Washington	Precision Crosslinking: Identifying and Interpreting Crosslinks Originating from Photoactive Amino Acids in Less-Ordered Regions of Proteins
7	Butalewicz, Jamie	UT Austin	Thermodynamic and Structural Characterization of the Main Protease of SARS-CoV-2 and Potential Inhibitors
8	Cain, Rebecca	IUPUI	Elucidation of Denatured Protein Structures in Solution and the Gas Phase Using Electrospray Ionization Mass Spectrometry Coupled with Crosslinking
9	Christofi, Emilia	U. Manchester	Use of Hybrid Mass Spectrometry methods to probe the structural flexibility of monoclonal antibody biotherapeutics across their production line
10	Constabel, May	U. Washington	Programmable, Temperature-Controlled ESI Enables Online Thermal Cycling and Disulfide Bond Reduction of Proteins
11	Cupp-Sutton, Kellye	U. Oklahoma	Investigation of the Effect of Staurosporine Induced Kinase Inhibition on HeLa using Top-down Proteome Profiling and Thermal Proteome Profiling
12	Dunham, Sean	UT Austin	Post UVPD Fractionation and PTCR reveals the deleterious impact of an abundant precursor ion in top down analysis of intact proteins (29-50 kDa)
13	Escobedo, Alesi	U. Washington	Standardization of Gas-phase Hydrogen/Deuterium Exchange for Resolving Isomeric Carbohydrate Anions
14	Evans, Kacie	TAMU	Improving Ion Activation on a 1.5 m Fourier Transform Ion Mobility (FT-IM) Orbitrap using a Segmented Quadrupole
15	Fan, Liqi	TAMU	Structurally Divergent Proteins Studied by Ion Mobility Mass Spectrometry: Human Metallothionein
16	Feng, Jiaxin	TAMU	In Situ Accurate Quantitative Mass Spectrometry Profiling of Isomeric Lipids via Aziridine-based Isobaric Tags Reveals Distinct Spatial Lipids Change in Medulloblastoma Mice
17	Gadallah, Mohamed	UT Austin	Structural Characterization of Pertussis Therapeutic Monoclonal Antibodies: Decoding Their Interactions with Antigens Via Native Mass Spectrometry
18	Gallagher, Elyssia	Baylor U	Modelling Protein Charging during Electrospray
19	Ghose, Shourjo	Bruker	Optimizing dia-PASEF isolation window schemes for proteomics measurements on a timsTOF ultra instrument
20	Gozzo, Theresa	U. Washington	A New Paradigm for Predicting Arrival-Time Distributions from Ion Mobility: Progress Towards a Statistical Treatment of Ion Transport
21	Gurav, Ankita	IUPUI	Structural Elucidation of Phosphorylated Alpha-Synuclein using Ion-Mobility Mass Spectrometry
22	Guttman, Mike	U. Washington	Orthogonal MS approaches for structural characterization of glycoconjugates
23	Harville, Payten	Yale	High-resolution vibrational predissociation spectroscopy of iodide-water by single-mode CW infrared excitation in a 3D cryogenic ion trap
24	Helms, Amanda	U Texas Austin	Top-Down Characterization of Histone Proteoforms with Capillary Electrophoresis-Tandem Mass Spectrometry using 193 nm UVPD
25	Jacinto, Jorge	UCSD	Using IC-FPOP to Understand the Molecular Mechanisms Causing Racial Health Disparities in Triple Negative Breast Cancer
26	Jeacock, Kiani	U Michigan	pH-dependent Oligomeric States of Bacterial Microcompartment Components
27	Jemison, Kezia	UCSD	Applying an Optimized Automated Workflow to FPOP Labeled Sample Handling and MS Analysis for Proteome-Wide Structural Biology
28	Jeon, Chae Kyung	U Michigan	Integrative modeling of individual particle tomography antibody models reveals gas-phase structural diversity and memory effects

29	Juetten, Kyle	U Texas Austin	Trapped Ion Mobility Spectrometry and UVPD for Probing the changes in Gas-Phase Native-like Protein Structure upon Crown Ether Complexation
30	Kirsch, Zachary	U. Massachusetts	Thrombin-DNA Aptamer Binding Investigated by DEPC Covalent Labeling-MS
31	Kostelic, Marius	Ohio State U	Characterization of PROTAC Ternary Complex Strength with Ion Mobility and Surface Induced Dissociation
32	Kuo, Alex	TAMU	Investigating SARS-CoV-2 Main Protease Dimerization Kinetics and Effects of Inhibitors by Native and Hydrogen Deuterium Exchange Mass Spectrometry
33	Kobal, Kari	MOBILion Systems	Tackling Citrullination and Deamidation Challenges in Proteomics using High - Resolution Ion Mobility-Mass Spectrometry
34	Lantz, Carter	TAMU	Digital Quadrupole Isolation and Electron Capture Dissociation on a Q-TOF-based Instrument Provides Sequence and Structure Information on Native Protein/Ligand Complexes
35	Prell, James	U. Oregon	The Physics of Multiple Collision Induced Dissociation and Unfolding: Design Principles Learned from an Improved Impulsive Collision Model

Tuesday Posters

36	Lanzillotti, Michael	U.Texas Austin	Analysis of Nucleic Acids by Online Buffer Exchange and m/z Domain Tandem-MS Fragment Identification
37	Ledesma, Pete	U. Minnesota	Evaluating the Impact of Unnatural Amino Acids on Structural Stability of Proteins
38	Lee, Jusung	U Florida	Differentiation of isomeric, non-separable carbohydrates using Tandem Trapped Ion Mobility Spectrometry–Mass Spectrometry (tandem-TIMS/MS)
39	Loo, Rachel	UCLA	Native Top-Down Mass Spectrometry: Proteins Ejecting, Dancing, and Rearranging
40	Luo, Haolin	UCSD	FragPipe for Proteome-Wide FPOP Analysis of Drug Target Engagement
41	Makey, Devin	U Michigan	Recommendations for Improved Native Mass Spectrometry Using Cyclic Ion Mobility-Mass Spectrometry
42	Mandapakar, Hyma	Wichita State U	Mapping Interacting Proteins of P53 C-terminal Domain Using New Asp/Glu-Targeting Chemical Cross-linkers
43	Marte, Joseph	U Michigan	IM-MS Reveals Structural Differences in α -Synuclein-Drug Complexes within Lipid Nanodiscs
44	Marty, Michael	U. Arizona	Identifying Membrane Protein-Lipid Interactions with Lipidomic Lipid Exchange-Mass Spectrometry
45	Martynova, Alice	U. Washington	Solving the Ligand Puzzle: Native Mass Spectrometry and Counting Ligands Bound to Fatty Acid Binding Proteins
46	Matney, Rowan	U. Minnesota	Benchmarking surface induced dissociation en route to “complex-down” gas-phase protein unfolding
47	Moeller, William	Ohio State U	Variable-Temperature Electrospray MS for Quantifying Protein-Ligand Cooperativity
48	Morris, Jalah	UCSD	Vascularized Organoids: An In-Cell Protein Footprinting Model for Human Disease
49	Moss, Olivia	Yale	Capture and Characterization of Nascent UV Photodecomposition Products with Mass-Selective Cryogenic Trapping Techniques
50	Newnham, Hari	U Manchester	Using Ion Mobility–Mass Spectrometry to aid the mechanistic understanding of [4Fe-4S] cluster assembly on the scaffold protein NUBP1
51	Oliva, Luis	UCSD	Using HDX-MS and FPOP as Complementary Methods To Identify Specific Binding Between NFkB-IkBa
52	Panda, Aniruddha	Yale	Direct determination of membrane protein complexes from proteoliposomes and cellular membranes using lipid bilayer native mass spectrometry platform and its applications
53	Papoulas, Ophelia	U. Texas Austin	A Ciliary Interactome Through Crosslinking Mass Spectrometry

54	Person, Maria	UT Austin	Mass Spectrometry Based Template-Assisted De Novo Sequencing of SARS-CoV-2 and Influenza Monoclonal Antibodies
55	Pizzala, Nicholas	Purdue U.	Ion Parking in Native MS: Spectral Decongestion, Signal Concentration, and Mass Determination
66	Ren, Hanlin	UT Austin	Characterization of a Nucleotide-Binding Site at C-Terminal Domain of Human TRAP1 by Native Mass Spectrometry and Ultraviolet Photodissociation
57	Rider, Robert	TAMU	Probing Protein Conformation using Variable-Temperature Electrospray Ionization
58	Ross, Imani	UCSD	Establishing CellROX Red as a Radical Dosimeter for Fast Photochemical Oxidation of Proteins (FPOP)
59	Roush, Addison	U. Washington	Next-Generation Ion Mobility Experiments Take a Long Time: Will Protein Ions Endure?
60	Sun, Liangliang	Michigan State U	Capillary electrophoresis-mass spectrometry for proteoforms
61	Sun, He Mirabel	TAMU	Native Mass Spectrometry Dissects the Details behind Individual ATP-GroEL Binding Steps
63	Vallejo, Daniel	Georgia Tech	Unlocking the Structural Information for Proteins Relevant to Cultural Heritage with Native and Top-Down Mass Spectrometry
64	Walker, Jada	U. Texas Austin	Structural elucidation of the 20S Proteasome using native ultraviolet photodissociation mass spectrometry
65	Wei, Ben	UCLA	Internal Fragments Enhance Middle-down Mass Spectrometry Structural Characterization of Monoclonal Antibodies and Antibody-drug Conjugates
66	Willelts, Matthew	Bruker	Single cell analysis with the label-free proteoCHIP and the Evotip adapter for high sensitivity proteomics on the timsTOF SCP
67	Wu, Oliver	U Oklahoma	HDX-MS with integrated protein thermal depletion (PTD) for elucidation of protein-ligand interactions in cell lysates
68	Yan, Yan	Stowers Institute	Revealing tissue-selective conformation and function of common proteome by multidimensional crosslinking profiling
69	Zhao, Boyu	UCLA	Native Top-Down MS with Orbitrap-Based Electron Capture Dissociation Reveals Higher Order Structure Information for Protein Complexes