

Speakers – please arrive ½ hour before your session begins to load your presentation

THURSDAY, JANUARY 25

4:00 - 7:00 pm **Setup all posters**, *Grand Bay Ballroom South*

6:00-7:00 pm **Registration**

7:00 - 8:00 pm Plenary Lecture <i>Grand Bay Ballroom North</i>
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7:00-7:15 pm **Opening Remarks**, Iain Campuzano, Frank Sobott and Michael Van Stipdonk

7:15-8:00 pm **PLENARY LECTURE: Jim Cheeseman**, *Gaussian, Inc.*
Quantum Mechanical Calculations: From Small Molecules to Helical Peptides

8:00-10:00 pm Reception <i>Grand Bay Ballroom South</i>

**The following students received an ASMS Student Travel Award.
Congratulations!**

Julian Bender
Martin Luther University Halle-Wittenberg,
Germany

Matthew Campbell
University of North Carolina

Rebecca D'Esposito
University at Albany

Sugyan Dixit
University of Michigan

Berkley Ellis
Vanderbilt University

Alexander Haack
University of Wuppertal, Germany

Neelam Khalan
Indiana University

Andy Lau
King's College, UK

Luke Metzler
Duquesne University (Advisor: Sherman)

Salahuddin Mohammad
Uppsala University, Sweden

Abhigya Mookherjee
University of Washington

Erin Panczyk
The Ohio State University

Amanda Patrick
NRC/AFRL

Elettra Piacentino
Northern Illinois University

Jordan Rabus
University of Missouri, St. Louis

Irena Tatosian
Duquesne University (Advisor: Van Stipdonk)

Alice Walker
University of North Texas

Natalia Yalovenko
EPFL, Switzerland

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FRIDAY, JANUARY 26

7:00 - 8:30 am **Continental Breakfast**, *Grand Bay Ballroom South*

8:30-11:00 am

Small Molecule and Protein Molecular Dynamics and Quantum Mechanics: The Basics

Session Chair: TBD

- 8:30-9:00 am **Adrian Roitberg**, *University of Florida*
Accuracy and Speed in Molecular Dynamics Simulations of Biomolecules
- 9:00-9:30 am **Michael Bartberger**, *Amgen, Inc.*
Applying MD and QM for Rational Drug Design
- 9:30-10:00 am **Beibei Wang**, *University of Calgary*
The Course-Grain Martini Force Field and Its Application for Membrane Protein Systems

10:00-10:15 am **Coffee Break**, *Grand Bay Ballroom South*

10:15-11:45 am

Small Molecule and Peptide Molecular Dynamics and Quantum Mechanics

Session Chair: Benjamin Bythell

- 10:15-10:45 am **Béla Paizs**, *Bangor University Wales*
Exploring Peptide Fragmentation Reactions Using Density Functional Theory Calculations
- 10:45-11:15 am **William Hase**, *Texas Tech University*
Chemical Dynamics Simulations of Peptide Ion Unimolecular Fragmentation and Collision-Induced Dissociation
- 11:15-11:45 am **Mary Rodgers**, *Wayne State University*
Synergistic Tandem MS and Theoretical Studies of Nucleic Acid Building Block Structure and Stability
- 11:45-Noon **Group Photo**
- Noon - 1:00 pm **Lunch and Learn Workshop Small Molecule Geometry Optimizations and CCS Calculations** (*provided by ASMS*)
Grand Bay Ballroom North

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FRIDAY, JANUARY 26

1:00-3:45 pm

**Computational Methods for Determination of Ion Structure
by Tandem Mass Spectrometry, Ion Mobility and Ion Spectroscopy**

Session Chair: Robert Continetti

Grand Bay Ballroom North

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| 1:00-1:30 pm | Ryan Steele , <i>University of Utah</i>
Vibrational Signatures of Electronic Properties in Molecules |
| 1:30-2:00 pm | Anne McCoy , <i>University of Washington</i>
Theoretical and Computational Approaches for Investigation of Molecules and
Complexes that Undergo Large Amplitude Vibrational Motions |
| 2:00-2:30 pm | Bert de Jong , <i>Lawrence Berkeley National Laboratory</i>
Application of High-Level DFT and QM-MD to Studies of Metal Ion Complexes |
| 2:30-2:45 pm | Coffee Break , <i>Grand Bay Ballroom South</i> |
| 2:45-3:15 pm | Steven Valentine , <i>West Virginia University</i>
Advanced Protocols for Molecular Dynamics Simulations and Collision Cross-Section
Calculation |
| 3:15-3:45 pm | Keith Richardson , <i>Waters Corporation, UK</i>
ETD Reagent Design for a Glow Discharge Source |

3:45-4:15

Hot Topic Talks

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| 3:45-4:00 pm | Natalia Yalovenko , <i>EPFL, Switzerland</i>
Poster # 37, Structural Determination of GRGDS and SDGRG by Combining Mass
Spectrometry, Ion Mobility, and Cryogenic Ion Spectroscopy |
| 4:00-4:15 pm | Styliani Consta , <i>University of Western Ontario, Canada</i>
Poster # 7, What Factors Determine the Stability of Weak Protein–Protein Interactions
in a Charged Aqueous Droplet |
| 4:15-7:00 pm | Free Time |

Speakers – please arrive ½ hour before your session begins to load your presentation

FRIDAY, JANUARY 26

7:00-8:30 pm

KEYNOTE LECTURE and Poster Flash Talks

Session Chair: Michael Van Stipdonk

Grand Bay Ballroom North

- 7:00-8:00 pm **KEYNOTE LECTURE: Mark Johnson, Yale University**
Experimental and Theoretical Investigation of Shared Protons in Water
- 8:00-8:30 pm **Seven Poster Flash Talks** (3 min each plus 1 min transition)
- Mohamed Alajmi, King Saud University, Saudi Arabia**
Poster # 1, Understanding the Interaction between Schiff base-based Anticancer Metal Complexes and Human Serum Albumin: a Spectroscopic and Molecular Docking Study
- Matthew Campbell, UNC**
Poster # 5, Exploring the Vast Conformational Space of Hexoses, Hexosamines, and N-acetylhexosamines with DFT and its Applications to Ion-Molecule Reactions
- Vinicius Wilian Cruzeiro, University of Florida**
Poster # 9, Applying Theoretical Modeling to Help the Interpretation of Ion Mobility/Mass Spectrometry Experiments: the Case of Cation-Dependent 25-Hydroxyvitamin D3 Conformations
- Rebecca D'esposito, University at Albany**
Poster # 11, A New Framework for the Coarse-Grained Simulation of Modified RNA
- Giorgis Isaac, Waters Corporations**
Poster # 17, Building a Collision Cross Section Library of Small Molecule Compounds Using an IMS QTOF Platform
- Rachel O. Loo, UCLA**
Poster # 21, Opposing Charges in ESI-MS of Noncovalent Complexes Explain Many Observations
- Erin Panczyk, The Ohio State University**
Poster # 25, Structural Influence of Dimethylproline Substitution on the Formation of b₂⁺ Ions by Gas-Phase Peptide Fragmentation

8:30-10:00 pm

**Poster Session I & Reception
Odd-Numbered Posters Present**

Grand Bay Ballroom South

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SATURDAY, JANUARY 27

7:00 - 8:30 am **Continental Breakfast, Grand Bay Ballroom South**

8:30-10:00 am
Computational Methods for Studies of Ion Chemistry
Session Chair: Christian Bleiholder
Grand Bay Ballroom North

8:30-9:00 am **Peter Armentrout, University of Utah**
Computational and Experimental Studies of Intrinsic Metal Ion Chemistry

9:00-9:30 am **Lai-Sheng Wang, Brown University**
Probing the Electronic Structure of Metal Complexes and Redox Species Using DFT and Anion Photoelectron Spectroscopy

9:30-10:00 am **Robert Continetti, University of California, San Diego**
Studies of Transient Species Using Electronic Structure Calculations and Photoelectron-Photofragment Coincidence Techniques

10:00-10:15 am
Hot Topic Talk

10:00-10:15 am **Daiki Asakawa, AIST, Japan**
Poster # 2, Fundamental Study of Hydrogen Attachment/Abstraction Dissociation (HAD) Tandem Mass Spectrometry by Ab initio Calculation

10:15-10:30 am **Coffee Break, Grand Bay Ballroom South**

10:30 -12:00 pm
Gas-Phase Structure and Reactions of Nucleic Acids and Glycans
Session Chair: TBD

10:30-11:00 am **Dan Fabris, University of Albany, SUNY**
Implementation of Course-Grain MD and Ion Mobility for Nucleic Acid Gas-Phase Structure Determination

11:00-11:30 am **Benjamin Bythell, University of Missouri, St. Louis**
DFT Study of Glycan Dissociation

11:30-12:00 pm **Valerie Gabelica, IECB, France**
All Atom MD and QM Calculations in Native Nucleic Acid MS and IM

10:00-10:15 am
Hot Topic Talk

12:00-12:15 pm **Neelam Khanal, Indiana University**
Poster # 16, Glycoanalysis with Cold Ion Spectroscopy and Ion Mobility: Studies of Glycosaminoglycans and Human Milk Oligosaccharides

12:15-1:45 pm, **Lunch and Learn Workshop: Macromolecular Modelling with Cross-Linking and Ion Mobility MS**, lunch is available for purchase in [online registration](#) (advance only). Cost is \$30.

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SATURDAY, JANUARY 27

1:45-4:00 pm

Protein-Ligand and Protein/Protein Complexes: Soluble and Membrane Proteins

Session Chair: Iain Campuzano

Grand Bay Ballroom North

- 1:45-2:15 pm **Thanh Do**, *University of Illinois, Urbana-Champaign*
The Application of MD and IM to Determine Structural Transitions from Solution to Gas-Phase
- 2:15-2:45 pm **Brandon Ruotolo**, *University of Michigan*
Using Course-Grain MD to Model Protein Sub-Unit Behavior in the Gas-Phase
- 2:45 -3:15 pm **Michael Marty**, *University of Arizona*
Pushing the Limits of Membrane Protein-Lipid Interactions with Nanodiscs, Native Mass Spectrometry, and MD
- 3:15-3:30 pm **Coffee Break**, *Grand Bay Ballroom South*
- 3:30-4:00 pm **Argyris Politis**, *Kings College, UK*
Modelling a Membrane Protein and its Interaction with Detergent Molecules in the Gas-Phase

4:00-4:30 pm

Hot Topic Talks

- 4:00-4:15 pm **Steffen Lindert**, *Ohio State University*
Poster # 20, Computational Protein Structure Prediction Guided by Covalent Labeling and SID Mass Spectrometry Data
- 4:15-4:30 pm **Andy Lau**, *Kings College, UK*
Poster # 18, Conformational Dynamics of the CSN-CRL2VBC~N8 Super Complex Revealed through cryo-EM and Hybrid Mass Spectrometry
- 4:30-7:00 pm **Free Time**

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SATURDAY, JANUARY 27

7:00-8:00 pm

KEYNOTE LECTURE and Poster Flash Talks

Session Chair: Frank Sobott

7:00-8:00 pm

KEYNOTE LECTURE: Perdita Barran, *University of Manchester, UK*
Using MD, MD and IM to Further Understand Protein Collapse in the Gas-Phase

8:00-8:30 pm

Seven Poster Flash Talks (3 min each plus 1 min transition)

J. Larry Campbell, *SCIEX, Canada*

Poster # 4, Using Differential Mobility Spectrometry and Machine Learning-Based Modeling to Predict Physicochemical Properties of Molecules

Yuri Corilo, *National High Magnetic Field Laboratory*

Poster # 6, Structural Determination of Polycyclic Aromatic Hydrocarbons by Ion Mobility Mass Spectrometry

David V. Dearden, *Brigham Young University*

Poster # 10, Computational and Experimental Studies of Gas Phase Container Complexes: Force Field Calculations Qualitatively Predict Extrusion Barriers

Abhigya Mookherjee, *University of Washington*

Poster # 24, Harnessing the Power of Ion Mobility and Orthogonal Mass Spectrometry-Based Techniques to Understand Glycan Fragmentation

Nicolas Polfer, *University of Florida*

Poster # 28, Solvent-Tagged Ions from Electrosprayed Solutions Probed by Gas-Phase IR Spectroscopy

Glenn Spangler, *Technispan LLC*

Poster # 32, Molecular Modeling and Interpreting IMS and IMS/MS Data

Irena Tatosian, *Duquesne University*

Poster # 34, Synthesis and Reactivity of [UO₂CO₂]⁻ Investigated Using Tandem Mass Spectrometry and Density Functional Theory Calculations

8:30-10:00 pm

Poster Session II & Reception

Even-Numbered Posters Present

Grand Bay Ballroom South

Speakers – please arrive ½ hour before your session begins to load your presentation

SUNDAY, JANUARY 28

7:00 - 8:30 am **Continental Breakfast**, *Grand Bay Ballroom South*

8:30-10:00 am

Ion Mobility Separation Algorithms: Which One is Optimal?

Session Chair: Michael Marty

Grand Bay Ballroom North

- 8:30-9:00 am **Carlos Larriba-Andaluz**, *Indiana University-Purdue University*
Molecular Dynamics/Kinetic Theory Algorithm for Numerical Determination of
Electrical Mobility
- 9:00-9:30 am **Christian Bleiholder**, *Florida State University*
Collision Cross Section Design and Considerations
- 9:30-10:00 am **Erik Marklund**, *Uppsala University, Sweden*
Computations for the Gas-Phase Study of Macromolecular Structure
- 10:00-10:15 am **Coffee Break**, *Grand Bay Ballroom South*

10:15-11:15 am

Molecular Dynamics and Quantum Mechanics in Medicinal Chemistry:

Real Therapeutic Case Studies

Session Chair: Brandon Ruotolo

- 10:15-10:45 am **Brian Lanman**, *Amgen, Inc.*
Application of MD, QM and SAR to Design a Peptide-Like Drug Targeting a Free
Cysteine Residue
- 10:45-11:15 am **Jens Meiler**, *Vanderbilt University*
Protein Structure Determination from Limited Restraints from Mass Spectrometry
- 11:15-11:30 am **Coffee Break**, *Grand Bay Ballroom South*

11:30 am-12:15 pm

KEYNOTE LECTURE and Closing Remarks

Session Chair: Rachel Loo

- 11:30-12:15 pm **KEYNOTE LECTURE: Lars Konermann**, *University of Western Ontario, Canada*
Modelling the Electrospray Processes by Molecular Dynamics
- 12:15-12:30 pm **Closing Remarks**, Iain Campuzano, Frank Sobott and Michael Van Stipdonk
- 12:30 pm **Remove all posters**