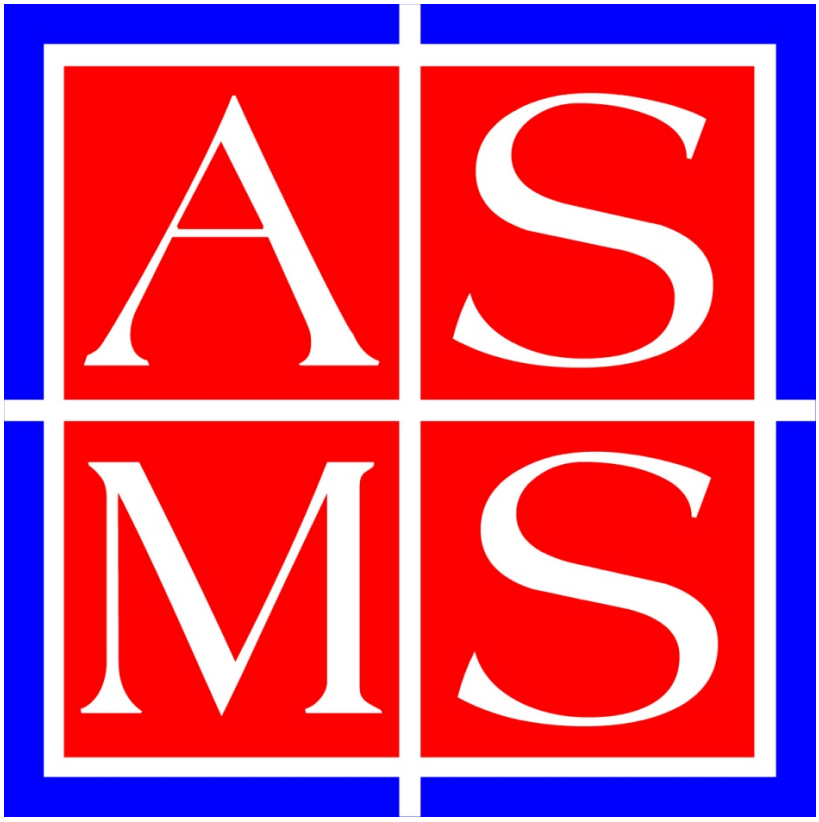

Computational Modelling in Mass Spectrometry and Ion Mobility: Methods for Ion Structure and Reactivity Determination

Organized by

Iain Campuzano
Amgen Inc.

Frank Sobott
University of Antwerp

Michael Van Stipdonk
Duquesne University

30th ASMS Sanibel Conference on Mass Spectrometry
January 25 - 28, 2018
St. Petersburg, FL

Thank you to our sponsors!

Waters

THE SCIENCE OF WHAT'S POSSIBLE.®

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
Grand Bay Ballroom North

7:00-7:15 pm **Opening Remarks**, Iain Campuzano, Frank Sobott and Michael Van Stipdonk

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

8:00-10:00 pm
Reception
Grand Bay Ballroom South

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

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

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: James R. Cheeseman

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 **Lucas Hamlow**, *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** *(lunch provided by ASMS)*
Grand Bay Ballroom North

Attendees will learn how to perform small molecule geometry optimization and charge fitting calculations using the Gaussian (commercial) and Firefly (free/academic) quantum mechanical programs, and how to use these results to calculate collisional cross section values using MOBCAL and IMoS.

Attendees are welcome (but not required) to follow along using their own laptops. If so, installation of the following programs is ahead of time are recommended:

- Avogadro (https://avogadro.cc) sketching and visualization program,
- Firefly (http://classic.chem.msu.su/gran/gamess/index.html)
- or Gaussian (http://gaussian.com) quantum chemistry program (if the attendee has a license for the latter)
- MOBCAL and IMoS CCS programs.

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

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

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

3:45-4:15
Hot Topic Talks

3:45-4:00 pm	**Natalia Yalovenko**, *EPFL, Switzerland* 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**, *University of Western Ontario, Canada* 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*
Mass Spec Meets FTIR: Where are we going with Optical Spectroscopies of Cryogenic Ions

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, Appling 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

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

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: Perdita Barran

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

12:00-12:15 pm
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

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

SATURDAY, JANUARY 27

12:15-1:45 pm **Lunch and Learn Workshop: Macromolecular Modelling with Cross-Linking and Ion Mobility MS,** *if you want a lunch you need to purchase it by 2:45 pm on Friday, cost is $30. You can also bring your own lunch.*
Grand Bay Ballroom South

In this workshop, attendees will learn how to source and prepare constituent subunits for modelling (MODELLER/PyMOL), generate topologies using cross-linking MS, prepare and submit protein complexes for gas phase simulation (GROMACS) and evaluate collision cross sections (IMPACT).

UNIX-based operating systems such as Linux and Mac OS are highly recommended for attendees wishing to follow the workshop on their own laptops. The following softwares are recommended for those wishing to participate in the tutorial (but are not essential as inputs and outputs of each section will be provided):

- MODELLER (https://salilab.org/modeller/)
- PyMOL (https://www.pymol.org/)
- GROMACS (http://www.gromacs.org/)
- IMPACT (http://impact.chem.ox.ac.uk/)

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*
Capturing Membrane Dynamics by Combining Structural Mass Spectrometry with Modelling

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**

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

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.*
Leveraging Biophysical and Computational Tools in the Design & Characterization of Covalent Peptidic Inhibitors of a Protein–Protein Interaction

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 Konerman,** *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**

POSTERS

Grand Bay Ballroom South
Setup up all posters by 7:00 pm on Thursday
ODD-numbered posters present during the Friday Poster Session
EVEN-numbered posters present during the Saturday Poster Session

1 **Understanding the Interaction between Schiff base-based Anticancer Metal Complexes and Human Serum Albumin: a Spectroscopic and Molecular Docking Study**; Mohamed Alajmi; *King Saud University, Riyadh, Saudi Arabia*.

2 **Fundamental Study of Hydrogen Attachment/Abstraction Dissociation (HAD) Tandem Mass Spectrometry by Ab initio Calculation**; Daiki Asakawa; *AIST, Tsukuba, Japan*.

3 **Structural Dynamics and Flexibility of the Neuronal Calcium-Sensor Synaptotagmin-1**; Julian Bender; *Interdisciplinary Research Center HALOmem, Martin Luther University Halle-Wittenberg, Halle (Saale), Germany*.

4 **Using Differential Mobility Spectrometry and Machine Learning-Based Modeling to Predict Physicochemical Properties of Molecules**; J. Larry Campbell; *SCIEX, Concord, ON*.

5 **Exploring the Vast Conformational Space of Hexoses, Hexosamines, and N-acetylhexosamines with DFT and its Applications to Ion-Molecule Reactions**; Matthew Campbell; *UNC, Chapel Hill, NC*.

6 **Structural Determination of Polycyclic Aromatic Hydrocarbons by Ion Mobility Mass Spectrometry**; Yuri Corilo; *National High Magnetic Field Laboratory, Tallahassee, FL*.

7 **What Factors Determine the Stability of Weak Protein–Protein Interactions in a Charged Aqueous Droplet?**; Styliani Consta; *University of Western Ontario, London, ON*.

8 **Lipids Shape the Electron Acceptor-Binding Site of the Peripheral Membrane Protein Dihydroorotate Dehydrogenase**; Joana Costeira-Paulo; *Uppsala University, Uppsala, Sweden*.

9 **Appling Theoretical Modeling to Help the Interpretation of Ion Mobility/Mass Spectrometry Experiments: the Case of Cation-Dependent 25-Hydroxyvitamin D3 conformations**; Vinicius Wilian Cruzeiro; *University of Florida, Gainesville, FL*.

10 **Computational and Experimental Studies of Gas Phase Container Complexes: Force Field Calculations Qualitatively Predict Extrusion Barriers**; David V. Dearden; *Brigham Young University, Provo, UT*.

11 **A New Framework for the Coarse-Grained Simulation of Modified RNA**; Rebecca D'esposito; *University at Albany, Albany, NY*.

12 **Studying Conformational Heterogeneity of Biomolecules Using Traveling Wave Ion Mobility Arrival Time Distributions and Molecular Dynamics Simulations**; Sugyan Dixit; *University of Michigan, Ann Arbor, MI*.

13 **Structural Characterization of Nonapeptide Diastereomers by Ion Mobility-Mass Spectrometry and Computational Models**; Berkley Ellis; *Vanderbilt University, Nashville, TN*.

14 **Thermodynamic and Kinetic Investigation of Proton Transfer Reactions between Amines and Solvent Clusters**; Alexander Haack; *University of Wuppertal, Wuppertal, Germany*.

15 **Coming Full Circle: A Computational Density Functional Investigation of Gas-Phase Ions Derived from Uranyl Benzoate and Halogenated Benzoate Precursors**; Cassandra Hanley; *Duquesne University, Pittsburgh, PA*.

16 **Glycoanalysis with Cold Ion Spectroscopy and Ion Mobility: Studies of Glycosaminoglycans and Human Milk Oligosaccharides**; Neelam Khanal; *Indiana University, Bloomington, IN*.

POSTERS

Grand Bay Ballroom South
Setup up all posters by 7:00 pm on Thursday
ODD-numbered posters present during the Friday Poster Session
EVEN-numbered posters present during the Saturday Poster Session

17 **Building a Collision Cross Section Library of Small Molecule Compounds Using an IMS QTof Platform**; Giorgis Isaac; *Waters Corporations, Milford, MA.*

18 **Conformational Dynamics of the CSN-CRL2VBC~N8 Supercomplex Revealed through cryo-EM and Hybrid Mass Spectrometry**; Andy Lau; *King's College London, United Kingdom*.

19 **Structure-Elucidation Using Tandem Trapped Ion Mobility Spectrometry-Mass Spectrometry (TIMS/TIMS-MS)**; Fanny Liu; *Florida State University*.

20 **Computational Protein Structure Prediction Guided by Covalent Labeling and SID Mass Spectrometry Data**; Steffen Lindert; *The Ohio State University, Columbus, OH*.

21 **Opposing Charges in ESI-MS of Noncovalent Complexes Explain Many Observations**; Rachel O. Loo; *UCLA, Los Angeles, CA.*

22 **Structure of the a1-Ion from Protonated, N-Terminus Derivatized Alanylglycine**; Luke Metzler; *Duquesne University, Pittsburgh, PA.*

23 **Single Analytical Method for Detecting Biomarkers of Migraine**; Salahuddin Mohammad; *Uppsala University, Uppsala, Sweden*.

24 **Harnessing the Power of Ion Mobility and Orthogonal Mass Spectrometry-Based Techniques to Understand Glycan Fragmentation**; Abhigya Mookherjee; *University of Washington, Seattle*.

25 **Structural Influence of Dimethylproline Substitution on the Formation of b2+ Ions by Gas-Phase Peptide Fragmentation**; Erin Panczyk; *The Ohio State University, Columbus, OH*.

26 **Proton Sharing and Transfer in Ionic Liquids Probed by Mass Spectrometry and Molecular Modeling**; Amanda Patrick; *NRC/AFRL, Albuquerque, NM*.

27 **Temperature Determination of Cryogenically Cooled Ion Traps Utilizing Rotationally Resolved I-(DOH) Vibrational Predissociation Spectroscopy**; Evan Perez; *Yale University, New Haven, CT*.

28 **Solvent-Tagged Ions from Electrosprayed Solutions Probed by Gas-Phase IR Spectroscopy**; Nicolas Polfer; *University of Florida, Gainesville, FL*.

29 **Gas-Phase Zinc-Based Catalysts for the Production of Hydrogen from Formic Acid**; Elettra Piacentino; *Northern Illinois University, Dekalb, Il.*

30 **Sweet and Sour: Anionic Sugar Acid Structure and Fragmentation Chemistry by Ion-Mobility Mass Spectrometry and Theoretical Methods**; Jordan Rabus; *University of Missouri, St. Louis, Saint Louis, MO*.

31 **Nonadiabatic Dynamics within the Fragmentation Pathways of Peptides**; Mary Sherman; *Duquesne University, Pittsburgh, PA.*

32 **Molecular Modeling and Interpreting IMS and IMS/MS Data**; Glenn Spangler; *Technispan LLC, Lutherville, MD*.

33 **Simulating Gas-Phase Amino Acids and Peptides in Combination with ESI-MS towards Probing Phosphopeptide Structure**; Anna Simmonds; *University of Birmingham, Birmingham, United Kingdom*.

POSTERS

Grand Bay Ballroom South
Setup up all posters by 7:00 pm on Thursday
ODD-numbered posters present during the Friday Poster Session
EVEN-numbered posters present during the Saturday Poster Session

34 **Synthesis and Reactivity of [UO2CO2]- Investigated Using Tandem Mass Spectrometry and Density Functional Theory Calculations**; Irena Tatosian; *Duquesne University, Pittsburgh, PA.*

35 **Multi-Microsecond Molecular Dynamics Simulations to Investigate the Unfolding of Hen Egg White Lysozyme in Ethanol in Combination with IMS-MS Studies**; Alice Walker; *University of North Texas, Denton, TX*.

36 **Interaction of Roundabout1-Ig1-2 and Heparan Sulfate Investigated by Ion Mobility and Molecular Dynamics**; Robert Williams; *University of Georgia, Athens, GA.*

37 **Structural Determination of GRGDS and SDGRG by Combining Mass Spectrometry, Ion Mobility, and Cryogenic Ion Spectroscopy**; Natalia Yalovenko; *EPFL, Lausanne, Switzerland*.

38 **Optimization of Long-Range Potential Interaction Parameters for CO2 and N2 Gases in Ion Mobility Spectrometry**; Tianyang Wu; *Purdue School of Engineering and Technology Mechanical Engineering, Indianapolis, IN*.

39 **Intrinsic Structures of Anionic Uranyl Nitrate Species Revealed by Tandem Mass Spectrometry, IRMPD Spectroscopy and DFT Calculations**; Amanda Bubas; *Duquesne University, Pittsburgh, PA.*

40 **Protein Modification across C3 to CAM Transition in *Mesombryanthemum crystallinum***, Theresa Kelley; *University of Florida, Gainesville, FL.*

41 **Mass Spectrometry for Determination of Peptide Abundance in Human Cancer Cell Lines Treated with Plant Extract**; Keyura Katam; *University of Florida, Gainesville, FL.*

42 **Identification of Defense-Related Proteins in Xylem of Disease Tolerant Grape Genotypes**; Tiffany Boynton; *Florida Agricultural and Mechanical University, Tallahassee, FL.*