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American Society for
Mass Spectrometry

ORGANIZERS

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IMPORTANT DEADLINES

November 29

Student and Post-doc
Travel Stipends

December 8

Abstracts for Posters and
Short Talks
Conference Registration

December 25

Hotel Reservations

30th SANIBEL CONFERENCE ON MASS SPECTROMETRY

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

January 25 - 28, 2018

Hilton St Petersburg • St. Petersburg, Florida

Molecular Dynamics (MD), Quantum Mechanical (QM) Calculations, Mass Spectrometry (MS) and Ion Mobility (IM) are all indispensable tools and biophysical measurement techniques used throughout a vast range of research topics within biopharmaceutical and academic research.

The combination of MD and QM with MS and IM has impacted multiple research fields: from small molecule structure-activity-relationship design, drug-protein docking experiments, fundamental gas-phase ion chemistries and reactivities, to structural characterization of small drug-like isomers, organometallics, large native protein complexes and even modelling of the electrospray process.

This conference will highlight contributions made by both established and new up-and-coming researchers in the field of MD, QM, MS and IM.

Keynote Speakers

- James Cheeseman, *Gaussian, Inc.*
- Mark Johnson, *Yale University*
- Perdita Barran, *University of Manchester*
- Lars Konermann, *University of Western Ontario*

Lunch and Learn Workshops

- **Friday:** Small Molecule Geometry Optimisations and CCS Calculations, *lunch provided by ASMS*
- **Saturday:** Macromolecular Modelling with Cross-Linking and Ion Mobility MS, *lunch is available for purchase*

PRELIMINARY PROGRAM (check www.asms.org for program updates)

Thursday, January 25, 2018

7:15-8:00 pm, **Plenary Lecture:** James Cheeseman, *Gaussian, Inc.*; "Quantum Mechanical Calculations: From Small Molecules to Helical Peptides"
8:00-10:00 pm, Reception

Friday, January 26, 2018

8:30-10:00 am, **Small Molecule and Protein Molecular Dynamics and Quantum Mechanics: The Basics**

- Romelia Salomon, *Pfizer*; "Using MD to Accurately Compute Protein Structure: Real-Life Protein Examples"
- Michael Bartberger, *Amgen Inc.*; "Applying MD and QM for Rational Drug Design"
- Beibei Wang, *University of Calgary*; "The Course-Grain Martini Force Field and Its Application for Membrane Protein Systems"

10:15-11:35 am, **Small Molecule and Peptide Molecular Dynamics and Quantum Mechanics**

- Béla Paizs, *Bangor University Wales*; "Exploring Peptide Fragmentation Reactions Using Density Functional Theory Calculations"
- William Hase, *Texas Tech University*; "Computer Simulations of Unimolecular and Intramolecular Dynamics"
- Mary Rodgers, *Wayne State University*; "Synergistic Tandem MS and Theoretical Studies of Nucleic Acid Building Block Structure and Stability"
- 20 minute Hot Topic Talk selected from contributed abstracts

11:35 am-1:00 pm, **Lunch and Learn Workshop: Small Molecule Geometry Optimizations and CCS Calculations**, *lunch provided by ASMS*

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.

1:00-3:00 pm, **Computational Methods for Determination of Ion Structure by Tandem Mass Spectrometry, Ion Mobility and Ion Spectroscopy**

- Ryan Steele, *University of Utah*; "Vibrational Signatures of Electronic Properties in Molecules"
- Anne McCoy, *University of Washington*; "Theoretical and Computational Approaches for Investigation of Molecules and Complexes that Undergo Large Amplitude Vibrational Motions"
- Bert de Jong, *Lawrence Berkeley National Laboratory*; "Application of High-Level DFT and QM-MD to Studies of Metal Ion Complexes"
- Steven Valentine, *West Virginia University*; "Advanced Protocols for Molecular Dynamics Simulations and Collision Cross-Section Calculation"
- Keith Richardson, *Waters Corporation, UK*; "ETD Reagent Design for a Glow Discharge Source"
- 20 minute Hot Topic Talk selected from contributed abstracts

Contact ASMS 505-989-4517 office@asms.org www.asms.org

PRELIMINARY PROGRAM (continued)

3:00-7:00 pm, Free Time

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, Six highlighted poster presentations (4 minute talks + 1 minute transition)

8:30-10:00 pm, Poster Session I

Saturday, January 27, 2018

8:30-10:10 am, **Computational Methods for Studies of Ion Chemistry**

- Peter Armentrout, *University of Utah*; "Computational and Experimental Studies of Intrinsic Metal Ion Chemistry"
- Lai-Sheng Wang, *Brown University*; "Probing the Electronic Structure of Metal Complexes and Redox Species Using DFT and Anion Photoelectron Spectroscopy"
- Robert Continetti, *University of California-San Diego*; "Studies of Transient Species Using Electronic Structure Calculations and Photoelectron-Photofragment Coincidence Techniques"
- 20 minute Hot Topic Talk selected from contributed abstracts

10:30-12:15 pm, **Gas-Phase Structure and Reactions of Nucleic**

Acids and Glycans

- Dan Fabris, *University at Albany, SUNY*; "Implementation of Course-Grain MD and Ion Mobility for Nucleic Acid Gas-Phase Structure Determination"
- Benjamin Bythell, *University of Missouri at St. Louis*; "DFT Study of Glycan Dissociation"
- Valerie Gabelica, *IECB, France*; "All Atom MD and QM Calculations in Native Nucleic Acid MS and IM"
- 20 minute Hot Topic Talk selected from contributed abstracts

12:15-1:45 pm, **Lunch and Learn Workshop: Macromolecular Modelling with Cross-Linking and Ion Mobility MS**, lunch is available to purchase in advance via registration (\$30)

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).

1:45-4:15 pm, **Protein-Ligand and Protein/Protein Complexes: Soluble and Membrane Proteins**

- Thanh D Do, *University of Illinois at Urbana-Champaign*; "The Application of MD and IM to Determine Structural Transitions from Solution to Gas-Phase"

- Brandon Ruotolo, *University of Michigan*; "Using Course-Grain MD to Model Protein Sub-unit Behavior in the Gas-Phase"
- Michael Marty, *University of Arizona*; "Pushing the Limits of Membrane Protein-Lipid Interactions with Nanodiscs, Native Mass Spectrometry, and MD"
- Argyris Politis, *Kings College, London, UK*; "Modelling a Membrane Protein and its Interaction with Detergent Molecules in the Gas-Phase"
- 2 x 15 minute Hot Topic Talks selected from contributed abstracts

4:15-7:00 pm, Free Time

7:00-8:00 pm, **Keynote Lecture:** Perdita Barran, *University of Manchester, UK*; "Using MD, MS and IM to Further Understand Protein Collapse in the Gas-Phase"

8:00-8:30 pm, Six highlighted poster presentations (4 minute talks + 1 minute transition)

8:30-10:00 pm, Poster Session II

Sunday, January 28, 2018

8:30-9:30 am, **Ion Mobility Separation Algorithms: Which One is Optimal?**

- Carlos Larriba-Andaluz, *Indiana University-Purdue University*; "Molecular Dynamics/Kinetic Theory Algorithm for Numerical Determination of Electrical Mobility"
- Christian Bleiholder, *Florida State University*; "Collision Cross Section Design and Considerations"
- Erik Marklund, *Uppsala University, Sweden*; "Computations for the Gas-Phase Study of Macromolecular Structure"

9:45-11:15 am, **Molecular Dynamics and Quantum Mechanics in Medicinal Chemistry: Real Therapeutic Case Studies**

- Brian Lanman, *Amgen*; "Application of MD, QM and SAR to Design a Peptide-Like Drug Targeting a Free Cysteine Residue"
- Jens Meiler, *Vanderbilt University*; "Application of Molecular Dynamics Simulations to Studies of Protein Conformational Change"
- 2 x 15 minute Hot Topics Talks selected from contributed abstracts

11:15-12:00 pm, **Keynote Lecture:** Lars Konermann, *University of Western Ontario*; "Modelling the Electrospray Processes by Molecular Dynamics"

12:00-12:15 pm, Closing Remarks: Iain Campuzano, Michael van Stipdonk and Frank Sobott

ABSTRACT SUBMISSION FOR POSTERS AND SHORT TALKS

A limited number of posters and short talks will be selected for oral presentations, please submit your abstract by **December 8**. The Sanibel Committee and the conference organizers reserve the right to reject an abstract which is judged to be inappropriate or which promotes a commercial or personal interest perspective.

To submit your abstract go to <http://www.asms.org/conferences/sanibel-conference/abstract-submission>

GENERAL INFORMATION

HILTON ST. PETERSBURG

The conference will be at the Hilton St. Petersburg, 333 1st Street South, St. Petersburg, FL. A block of guest rooms for conference attendees is available at the special rate of \$189/night plus tax. Wifi is included in all ASMS guest rooms. To reserve your room, go to <http://www.asms.org/conferences/sanibel-conference/lodging-travel>. **Deadline for reservations is December 25**. Don't be disappointed, reserve your room early!

OFFSITE PARTICIPANT FEE

If you choose not to stay at the Hilton St. Petersburg, you must pay the offsite participant fee of \$200. The offsite fee may be paid at online registration or using the enclosed registration form.

TRAVEL TO ST. PETERSBURG

There are two nearby airports, Tampa International Airport (TPA), the main airport and St. Petersburg/Clearwater Airport (PIE). Conference registrants may opt to take a taxi, ride with a shared van service, or rent a car at the airport. For more information visit <http://www.asms.org/conferences/sanibel-conference/lodging-travel>.

STUDENT AND POST-DOC TRAVEL STIPENDS

Twenty stipends of up to \$750 each available to students and post-docs within two years of first appointment. Stipend recipients will also receive complimentary registration. Deadline is November 29.

Applications are completed and submitted online only. Complete eligibility and application details available at www.asms.org/conferences/sanibel/student-post-doc-travel-stipends.

ASMS SANIBEL CONFERENCE REGISTRATION FORM

DEADLINE: DECEMBER 8

ONLINE REGISTRATION NOW AVAILABLE. To register quickly go to <http://www.asms.org/conferences/sanibel-conference/registration>. If needed, use the printable form below.

REGISTRATION DEADLINE IS DECEMBER 8. Use this form to register for the Conference and pay the offsite participant fee.

CANCELLATION. Written notice of cancellation must be received by January 17, 2018. \$50 will be deducted from refunds to cover the cost of processing.

Name		Institution	
Street Address			
City	State	Zip (or postal code)	Country
Business Phone		Email	

CONFERENCE REGISTRATION. Deadline is December 8. After December 8 registration fees will increase by \$50. Registration will remain open after December 8 on a space-available basis.

☐ ASMS Member, \$400 ☐ Non-Member, \$600 ☐ Student, \$175*

**Must be a full-time student in a degree program. Include copy of student ID.*

Enter registration amount \$ _____

ACCOMMODATIONS AT HILTON ST. PETERSBURG. Reserve your room at Sanibel online.
Deadline is December 25, 2017.

To reserve your room go to <http://www.asms.org/conferences/sanibel-conference/lodging-travel>.

SATURDAY LUNCH. Lunch on Saturday is not provided and is available to purchase in advance only.
Cost is \$30. *Note that Friday lunch is provided by ASMS at no extra charge.*

Saturday lunch, enter \$30 \$ _____

OFF-SITE PARTICIPANT FEE. Conference attendees who choose not to stay at the Hilton St. Petersburg must pay an offsite fee of \$200.

☐ Yes, I will reserve (have reserved) a room at Hilton St. Petersburg

☐ No, I will not stay at the Hilton. I will stay in an offsite motel.

If you are NOT staying at Hilton St. Petersburg, enter \$200 \$ _____

ENTER TOTAL AMOUNT \$ _____

PAYMENT. Please check payment method below.

☐ Check for the total amount payable in U.S. dollars is enclosed. Make check payable to ASMS. **Check must be payable through a bank with a U.S. address printed on the check.**

☐ Charge the total amount to credit card below.

Visa, MC, or AmEx Card Number	Exp Date	3 or 4 Digit Security Code
Cardholder's Name	Cardholder's Signature	



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