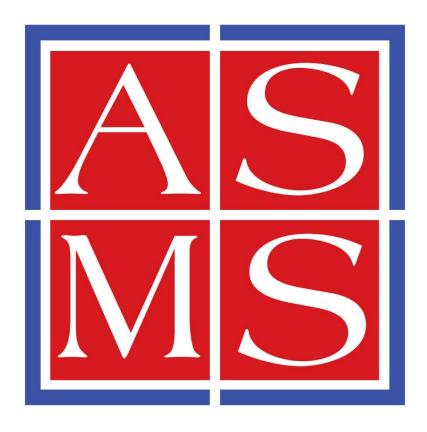
Your Name: _____



Membrane Proteins and Their Complexes: Mass Spectrometry and Beyond

Organized by

Michael T. Marty, *University of Arizona*, Wendy Sandoval, *Genentech* & Julian Whitelegge, *UCLA*

33rd Sanibel Conference on Mass Spectrometry January 19 – 22, 2023 Island Grand Tradewinds, Captiva, FL

THURSDAY, JANUARY 19

4:00 - 7:00 pm **Setup all posters**, *The Pavilion*

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

7:00 - 7:10 pm Opening Remarks, Michael T. Marty, Wendy Sandoval & Julian Whitelegge

The Pavilion

7:10 - 8:10 pm Keynote Lecture

Mass Spectrometry of Membrane Proteins in Complex with Lipids Art Laganowsky, Texas A&M University

Session Chair: Julian Whitelegge *The Pavilion*

8:10-10:00 pm Reception The Pavilion

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

Julia Hesselbarth

Johannes Gutenberg University Mainz

Virginia James

University of Texas at Austin

Brock Juliano

University of Michigan

Philip Lacey

The Ohio State University

Xiaoxuan Lin

The University of Chicago

Neil McCracken

Indiana University

Robert Schrader

Texas A&M University

Qianjie Wang

Michigan State University

Guozhi Zhang

The University of Arizona

FRIDAY, JANUARY 20

7:00 - 8:30 am **Continental Breakfast**, *The Pavilion*

8:30 - 9:30 am Membrane Protein Sample Preparation Session Chair: Oliver Hale		
	The Pavilion	
8:30 - 9:00 am	Native Top-Down Mass Spectrometry with Electrons and Collisions of Membrane Protein Complexes, Joseph Loo , <i>UCLA</i>	
9:00 - 9:30 am	Surface Induced Dissociation of Membrane Peptides and Proteins from Nanodiscs and Micelles, Vicki Wysocki , <i>Ohio State University</i>	
9:30 - 10:00 am	Coffee Break, The Pavilion	
10:00 am – 11:50 am Instrumentation Session Chair: Mowei Zhou		
10:00 - 10:20 am	Deorphanizing Tough Membrane Targets Using Recombinant Extracellular Vesicles, Shengya Cao , <i>Genentech</i>	
10:20 – 10:50 am	Hydrophobic Protein Analysis in Industry: From Native-MS to High Throughput-MS Therapeutic Project Support, Iain Campuzano , <i>Amgen</i>	
10:50 – 11:20 am	Membrane Protein Complexes and their Environments, Nina Morgner, Goethe University Frankfurt	
11:20 – 11:50 am	Developments in the Analysis of Membrane Proteins on Orbitrap Platforms, Rosa Viner , <i>Thermo Fisher Scientific</i>	
11:50 -12:05 pm	Group Photo	
12:05 - 1:15 pm	Group Lunch, provided by ASMS The Pavilion	

	1:15-2:15 pm
	Ion Mobility
	Session Chair: Kelly Hines
1:15 – 1:45 pm	Collision Induced Unfolding of Membrane Proteins and their Complexes, Brandon Ruotolo , <i>University of Michigan</i>
1:45 – 2:15 pm	Probing Gibbs Energy Landscape of Proteins: Variable Temperature-ESI and Ion Mobility-High Resolution Mass Spectrometry, David Russell , <i>Texas A&M University</i>
	2:15 - 2:55 pm Submitted Talks
	Session Chair: Kelly Hines
2:15 – 2:35 pm	Single Cardiomyocytes Membrane Protein Content, Jenny Van Eyk, Cedar Sinai Medicial Center
2:35 – 2:55 pm	Imaging Mass Spectrometry of Integral Membrane Proteins, Kevin Schey , <i>Vanderbilt University</i>
2:55 – 7:00 pm	Free Time
	7:00 – 8:20 pm Submitted Talks
	Session Chair: Fanny Liu
7:00 – 7:20 pm	Exploring the Pharmacology of GPCRs by Native MS Results in Identification of Endogenous Ions that Serve as Positive Allosteric Modulators, Idlir Liko, OMass Therapeutics
7:20 – 7:40 pm	High-level Daptomycin Resistance is Supported by Increased Membrane Fluidity in <i>Staphylococcus aureus</i> with Defective Phosphatidylglycerol Synthesis, Kelly Hines, <i>University of Georgia</i>
7:40 – 8:20 pm	Two-minute Flash Talks from the Odd-Numbered Posters, see Poster List on page 7

8:20-10:00 pm
Poster Session I & Reception
Odd-Numbered Posters Present
The Pavilion

SATURDAY, JANUARY 21

7:00 - 8:30 am **Continental Breakfast**, The Pavilion

7:30 - 8:30 am

Fully Integrated Native MS Workflow Discussion Panel, optional

Vicki Wysocki, Ohio State University The Pavilion

8:30 – 10:00 am **Membrane Mimetics**

Session Chair: Chloe Martens		
8:30 – 9:00 am	Native MS and Lipidomics for Measuring Membrane Protein-Lipid Interactions in Heterogeneous Nanodiscs, Michael T. Marty , <i>University of Arizona</i>	
9:00 – 9:30 am	Gabor Transform Tools for Mass Spectrometry Characterization of Nanodiscs and Membrane Proteins, James Prell , <i>University of Oregon</i>	
9:30 – 10:00 am	Integrative Structural Mass Spectrometry to Interrogate Amphipol-Protein Assemblies and Inform on the Molecular Mechanism of Outer Membrane Protein Biogenesis, Antonio Calabrese , <i>University of Leeds</i>	

10:00 - 10:30 am, Coffee Break

10:30 - 12:00 pm **Biophysical Characterization**

Session Chair: Carter Lantz

10:30 – 11:00 am	MS and EM - A Marriage Made in the Membrane?, Frank Sobott, University of Leeds
11:00 – 11:30 am	Unlocking the Functional Dynamics of Membrane Transporters by HDX-MS, Argyris Politis , <i>University of Manchester</i>
11:30 – 12:00 pm	Protein Interactions in Synaptic Vesicles and in the Neuronal Synapse Studied by Structural Mass Spectrometry, Carla Schmidt, HALOmem, Martin Luther University Halle-Wittenberg
12:00 - 1:30 pm	Lunch on your own

SATURDAY, JANUARY 21

	1:30 – 3:00 pm Proteomics Session Chair: Si Wu	
1:30 – 2:00 pm	How Does a Single Mutation in the Membrane Protein CFTR Cause the Disease Cystic Fibrosis, John Yates , <i>Scripps Research Institute</i>	
2:00 – 2:30 pm	Maintaining Higher-Order Structure while Removing Non-Covalent Associations for Effective Electrospray Ionization of Integral Membrane Proteins, Julian Whitelegge , <i>UCLA</i>	
2:30 – 3:00 pm	Ultraviolet Photodissociation for Analysis of Membrane Protein Complexes, Jennifer Brodbelt , <i>University of Texas</i>	
3:00 - 3:30 pm	Coffee Break	
3:30 – 4:50 pm Membrane Protein Structural Biology and Biophysics Session Chair: Wendy Sandoval		
3:30 – 3:50 pm	3D Structure Determination of Protein Complexes Using Matrix-Landing Mass Spectrometry, Josh Coon , <i>University of Wisconsin</i>	
3:50 – 4:20 pm	Transmembrane Helices Mediate the Formation of a Stable Ternary Complex Composed of Cytochrome b5, Cytochrome B5 Reductase and Stearoyl-Coa Desaturase-1, Ming Zhou , <i>Baylor College of Medicine</i>	
4:20 – 4:50 pm	Direct Determination of Organization of Membrane Protein and Lipids from Intact Customizable Lipid Bilayers, Kallol Gupta , <i>Yale University</i>	
	7:00 - 8:20 pm Submitted Talks II Session Chair: Melanie Odenkirk	
7:00 – 7:20 pm	Deciphering the Allosteric Regulation of the NBD1 Domain of CFTR Channel by HDX-MS and Single-Molecule FRET, Chloe Martens , <i>Université Libre de Bruxelles</i>	
7:20 – 7:40 pm	A Tailored Approach for the Analysis of Membrane Proteins from Tissue Using Native Nano-DESI Mass Spectrometry, Emma Sisley , <i>University of Birmingham</i>	
7:40 – 8:20 pm	2-minute Flash Talks from Even-Numbered Posters, see Poster List on page 7	

8:20-10:00 pm Poster Session II & Reception Even-Numbered Posters Present

The Pavilion

SUNDAY, JANUARY 22

7:00 - 8:30 am Continental Breakfast, The Pavilion

8:30-10:00 am Glycosylation and Lipids Session Chair: Fabio Gomes The Pavilion		
8:30 – 9:00 am	MS Support for Membrane Protein Efforts in Structural Biology, Wendy Sandoval, Genentech	
9:00 – 9:30 am	MS-Based Investigations of Social and Anti-Social Distancing at the Cell Surface, Cathy Costello , <i>Boston University School of Medicine</i>	
9:30 – 10:00 am	Fingerprinting the Unique Lipidome of Membrane Proteins, Erin Baker, North Carolina State University	

10:00 - 10:15 am, Coffee Break

10:15 – 11:15 am Keynote Lecture

Membrane Proteins in Context Carol Robinson, University of Oxford

Session Chair: Michael T. Marty *The Pavilion*

11:15 - 11:30 am Closing Remarks, Michael T. Marty, Wendy Sandoval and Julian Whitelegge

The Pavilion

- Mapping an Allosteric Response in a TonB Dependent Transporter Using Hydrogen Exchange in E. coli Outer Membranes; Michael C Baxa¹; Adam M. Zmyslowski^{1, 2}; Isabelle A Gagnon¹; Tobin R Sosnick¹; ¹University of Chicago, Chicago, IL; ²Evozyne LLC, Chicago, IL
- Charge Deconvolution and Peak Assignment for Native MS on Metal-Ion-Containing Complexes; Marshall W. Bern¹; Ignat Shilov¹; Christian Heckendorf¹; Yun Zhu²; David Russell²; Arthur D Laganowsky²; Protein Metrics, Cupertino, CA; Texas A&M University, College Station, TX
- 3 Structure Relaxation Approximation (SRA): A Framework for Elucidating Protein Structures with Ion Mobility Spectrometry; Christian Bleiholder¹; Mengqi Chai²; Fanny C Liu¹; ¹Florida State University, Tallahassee, FL; ²Washington University, Saint Louis, MO
- Automated Native Mass Spectrometry Screening of Membrane Proteins for Structural Biology Applications; Natalia De Val¹; Scott Kronewitter²; Paul Gazis³; Mick Greer⁴; Weijing Liu³; Rosa Viner³; Olufemi Adeyemi⁵; Albert Konijnenberg⁵; Thermo Fisher Scientific, Frederick, MD; Thermo Fisher Scientific, Cambridge, Massachusussetts; Thermo Fisher Scientific, San Jose, California; Thermo Fisher Scientific, Austin, TX; Thermo Fisher Scientific, Eindhoven, Netherlands
- 5 Structure and Stability of Human MT2A and Transthyretin Mutants: Gas-Phase and Solution-Phase; Liqi Fan¹; David H Russell¹; ¹Texas A&M University, College Station, TX
- 6 Elucidating Protein-Ligand Interactions in Cell Lysates Using High Throughput Hydrogen Deuterium Exchange Mass Spectrometry with Integrated Protein Thermal Depletion; Mulin Fang¹; Oliver Wu¹; Kellye A. Sutton¹; Si Wu¹; University of Oklahoma, Norman, OK
- 7 Understanding the Role of Estrogen Receptor-α Proteoforms and Their Complexoforms in the Membrane; Fabio P. Gomes¹; John R. Yates¹; The Scripps Research Institute, La Jolla, CA
- Analysis and Imaging of Aquaporin-0 Assemblies Directly from Eye Lens Tissue with nano-DESI; Oliver J Hale¹; Helen J Cooper¹; ¹University of Birmingham, Birmingham, United Kingdom
- A Roadmap for SNARE Complex Assembly: Mass Spectrometry Uncovers Intermediates and "Off-Pathway" Complexes; Julia Hesselbarth¹; Carla Schmidt¹; ¹Johannes Gutenberg University Mainz, Department of Chemistry Biochemistry, Mainz, Germany
- Monitoring the Preservation of Native Structure Throughout Mass Spectrometry

 Experiments Using Orbitrap Collision Cross Section Measurements; Virginia K James¹;

 Jennifer S. Brodbelt¹; ¹University of Texas at Austin, Austin, TX
- Mutant Cycle Analysis Reveals Membrane Protein-Lipid Interactions; <u>Hiruni S Jayasekera</u>¹; Megan Ewbank¹; Michael T Marty¹; ¹The University of Arizona, Tucson, AZ
- Development of Improved Methodologies for the Native Top-Down Mass Spectrometry of Transmembrane Proteins; Brock R Juliano¹; Brandon T Ruotolo¹; ¹University of Michigan, Ann Arbor, MI
- Characterizing Membrane Proteins with Mass Photometry and Membrane Mimetics;

 Gogulan Karunanithy¹; Zornitsa Kofinova¹; Caolan Browne²; Philip Kitchen²; Candice Mach³; Sofia Ferreira¹; ¹Refeyn, Oxford, United Kingdom; ²Aston University, Birmingham, United Kingdom; ³Refeyn, Boston, MA

The Pavilion

- Deciphering Solution and Gas Phase Interactions Using Native Mass Spectrometry; <u>Til Erik Kundlacz</u>¹; Carla Schmidt^{1,2}; ¹Martin-Luther-Universität Halle-Wittenberg, Interdisciplinary Research Center HALOmem, Institute for Biochemistry and Biotechnology, Halle (Saale), Germany; ²Johannes Gutenberg University Mainz, Department of Chemistry Biochemistry, Biocenter II, Mainz, Germany
- Electron Capture Charge Reduction Improves Resolution of Intact Nanodiscs in Native Mass Spectrometry; Philip C. Lacey, 2; Marius M Kostelic, Sophie R. Harvey, Jared B. Shaw⁴; Vicki H. Wysocki, The Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; Resource for Native MS Guided Structural Biology, The Ohio State University, Columbus, OH; Campus Chemical Instrumentation Center, The Ohio State University, Columbus, OH; Pe-MSion, Inc., Corvallis, OR
- Digital-Waveform Technology and Electron Capture Dissociation on a Q-TOF-based Instrument Provides Sequence and Structure Information on Native Protein Ions; Carter Lantz¹; Robert Schrader¹; David H Russell¹; Texas A&M University, College Station, TX
- A Critical Evaluation of Detergent Exchange Methodologies for Native Mass Spectrometry of Membrane Proteins; <u>Iliana Levesque</u>¹; Brock R. Juliano¹; Kristine F. Parson¹; Brandon T Ruotolo¹; ¹University of Michigan, Ann Arbor, MI
- Folding Stability at the Anion-Binding Site Distinguishes Motor Prestin from Its Homologous Anion Transporters as Revealed by HDX-MS; Xiaoxuan Lin¹; Patrick Haller¹; Navid Bavi¹; Nabil Faruk²; Eduardo Perozo¹,³; Tobin R Sosnick¹,⁴,⁵; ¹Department of Biochemistry and Molecular Biology, The University of Chicago, Chicago, IL; ²Graduate Program in Biophysical Sciences, The University of Chicago, Chicago, IL; ³Grossman Institute for Neuroscience, Quantitative Biology and Human Behavior, The University of Chicago, Chicago, Chicago, IL; ⁴Prizker School for Molecular Engineering, The University of Chicago, Chicago, IL; ⁵Institute for Biophysical Dynamics, The University of Chicago, Chicago, IL
- 19 **Proteome and Lipidome of Complex I Deficient Cells and Their Mitochondria**; <u>Vanessa Linke</u>^{1, 2}; Agnieszka Chacinska^{1, 2}; ¹Laboratory of Mitochondrial Biogenesis, IMol Polish Academy of Sciences, Warsaw, Poland; ²ReMedy International Research Agenda Unit, IMol Polish Academy of Sciences, Warsaw, Poland
- Towards Integrating Tandem-Trapped Ion Mobility Spectrometry/Mass Spectrometry, Collision-Induced Dissociation, and Parallel-Accumulation Serial Fragmentation for Top-Down Analysis of Viral Glycoproteins; Fanny C Liu¹; Thais Pedrete¹; Jusung Lee¹; Christian Bleiholder¹; Florida State University, Tallahassee, FL
- 21 **Structural Basis for Lipid and Copper Regulation of the ABC Transporter MsbA**; <u>Jixing Lyu</u>¹; Chang Liu²; Tianqi Zhang¹; Samantha Schrecke¹; Elam P. Nicklaus¹; Charles Packianathan¹; Georg K. A. Hochberg^{3, 4}; David Russell¹; Minglei Zhao; ¹Texas A&M University, College Station, TX; ²University of Chicago, Chicago, IL; ³Max Planck Institute for Terrestrial Microbiology and Department of Chemistry, University of Marburg, Marburg, Germany; ⁴Center for Synthetic Microbiology (SYNMIKRO), Department of Chemistry, University of Marburg, Marburg, Germany
- The (PERK)s of Understanding ER Stress: Characterizing a Transmembrane Sensor Linked with Diabetes Using MS-based Thermal Shift Assays; Neil Mccracken¹; Whitney Smith-Kinnaman¹; Stephane Pelletier¹; Ronald Wek¹; Amber Mosley¹; Indiana University, Indianapolis, IN

The Pavilion

- Affinity Selection Mass Spectrometry for Membrane Proteins; Philip Nevin; Astrazeneca, Molndal, Sweden
- Assessing the Influence of Nanodisc Assembly Conditions on the Uptake of Bacterial and Mammalian Lipid Extracts; Melanie Odenkirk¹; Guozhi Zhang¹; Michael T Marty¹; ¹University of Arizona, Tucson, AZ
- Deciphering Hierarchical Organization of Proteins & Lipids Involved in Neuronal Exocytosis Using Lipid Bilayer Native Mass Spectrometry; Aniruddha Panda^{1,2}; Kallol Gupta^{1,2}; ¹Yale Nanobiology Institute, West Haven, CT; ²Department of Cell Biology, New Haven, CT
- Non-Covalent Complexes Involving Cytochrome P450 Captured Within Lipid Nanodiscs Reveal Insights into P450-Containing System Drug Interactions; Kristine F Parson¹; Brandon T Ruotolo¹; ¹University of Michigan, Ann Arbor, MI
- Traffic-Generated Emissions Exposure and High-Fat Diet Consumption Alter Protein Expression Associated with Antioxidant Activity and Cell Death in C57Bl/6 Mice; Leah J Schneider^{1, 2}; Bea Penaredondo¹; Lanie Stanley¹; Yuan Lin³; David Butcher³; Lissa Anderson³; Amie K Lund¹; ¹University of North Texas, Denton, TX; ²CFD Research Corporation, Dayton, OH; ³National High Magnetic Field Laboratory, Tallahassee, Florida
- Modified Ion Source for Improved Collisional Activation of Protein Complexes; Robert L. Schrader¹; Thomas Walker¹; David H Russell¹; Texas A&M University, College Station, TX
- Mass Spectrometric Analysis of Charged Microdroplet-Mediated Cardiolipin-Cytochrome C Complex; Cheyenne P Sircher¹; Ashton Taylor¹; Theresa Evans-Nguyen¹; ¹University of South Florida, Tampa, FL
- Development of *in vivo* Hydrogen-Deuterium Exchange/MS with applications to a TonB-Dependent Transporter and Other Proteins; Xiaoxuan Lin¹; Adam M. Zmyslowski¹; Isabelle A Gagnon¹; Robert Nakamoto²; Tobin R Sosnick¹; ¹University of Chicago, Chicago, IL; ²University of Virginia, Charlettesville, VA
- Revealing the Driving Force for the Function of a mega-Dalton Chaperone by Native Mass Spectrometry; He M Sun¹; Thomas Walker²; David H Russell²; Arthur D Laganowsky²; ¹Texas A&M University, College Station, TX; ²Texas A&M University, College Station, TX
- Top-Down Proteomics Profiling of Membrane Proteins in Arabidopsis thaliana Leaf, Stem, and Root Tissues; Stephanie Thibert¹; Jesse Wilson¹; Vimal Balasubramanian¹; Deseree Reid¹; John Melchior^{1, 2}; Kim Hixson¹; Tanya Winkler¹; Roza Wojcik¹; Aivett Bilbao^{1, 1}Pacific Northwest National Laboratory, Richland, WA; ²University of Cincinnati, Cincinnati, OH
- Evaluation of Mitochondrial Content in Plasma Extracellular Vesicles; Ai Nguyen¹; <u>Illarion Turko</u>¹; <u>Institute for Bioscience and Biotechnology Research, Rockville, MD</u>
- Membrane Protein Structure and Binding Interactions in Cells Using Covalent Labeling Mass Spectrometry; Zachary J. Kirsch¹; Xiao Pan¹; Thomas Tran¹; Lynmarie K. Thompson¹; Eric M. Graban²; Robert C. Vaughan²; Richard Vachet¹; ¹University of Massachusetts Amherst, Amherst, MA; ²QuarryBio, Tallahassee, FL

The Pavilion

- Capillary Zone Electrophoresis Mass Spectrometry for Characterization of Membrane Proteins; Qianjie Wang^{1,2,3}; Peter Lundquist^{1,2}; Liangliang Sun³; ¹Department of Biochemistry and Molecular Biology, Michigan State University, East Lansing, MI; ²Plant Resilience Institute, Michigan State University, East Lansing, MI; ³Department of Chemistry, Michigan State University, East Lansing, MI
- Epitope mapping of Anthrax Protective Antigen (PA) in Human Serum Samples Using High Throughput HDX-MS; Si Wu; University of Oklahoma, Norman, OK
- Lipidomic Lipid Exchange Mass-Spectrometry (LX-MS) to Survery the Membrane Proteins Lipid Environment; Guozhi Zhang¹; Melanie T Odenkirk¹; Michael T Marty¹;

 IUniversity of Arizona, Tucson, AZ
- Novel Cleavable Surfactants for Top-down Proteomics of Membrane Proteins; Kyle Brown¹; Morgan Gugger¹; Bifan Chen¹; Tania Guardado¹; Ziqing Lin¹; David Moreno¹; Song Jin¹; Yanlong Zhu¹; Ying Ge¹; ¹University of Wisconsin-Madison, Madison, WI
- Cupric ions Selectively Modulate TRAAK-Phosphatidylserine Interactions; Yun Zhu¹; Samantha Schrecke¹; Shuli Tang¹; Melanie T Odenkirk²; Thomas Walker¹; Lauren Stover¹; Jixing Lyu¹; Tianqi Zhang¹; David H Russell¹; Erin S; ¹Texas A&M University, College Station, TX; ¹The University of Arizona, Tucson, AZ; ³The University of North Carolina at Chapel Hill, Chapel Hill, NC
- Role of Membrane Phospholipids in Flavor Development and Off-Odor Formation; <u>Joshua Zyzak</u>¹; Li Li Zyzak¹; ¹*Eastern Kentucky University, Richmond, KY*



UPCOMING EVENTS

George R. Brown Convention Center (GRB) | Houston, Texas

Abstract Deadline is February 3, 2023

More information at https://www.asms.org/conferences/annual-conference

October 13 - 17, 2023 38th Asilomar Conference on Mass Spectrometry Computational Mass Spectrometry

Asilomar Conference Center | Pacific Grove, CA

Organizers
Nuno Bandera, *UC, San Diego*, David Fenyo, *New York University* and Olga Vitek, *NEU*

2023 Fall Workshop

Lipidomics – The Essentials to the Cutting Edge

Date and Location TBD

Organizers

Timothy Garrett, University of Florida and Jace Jones, University of Maryland