

# LAKE LOUISE XXIX

## 29th Workshop on Tandem Mass Spectrometry

THURSDAY, DECEMBER 1

8:00 Introductory Remarks: *Lars Konermann*

**Ion Mobility MS/MS**      Chair: *Kristina Håkansson*

8:10 *Chris Hogan*, Department of Mechanical Engineering, University of Minnesota, Minneapolis, MN  
“Monitoring and Modeling Adsorption in the Gas and Liquid Phases via Ion Mobility Spectrometry”

8:35 *Matt Bush*, Department of Chemistry, University of Washington, Seattle, WA  
“Cation-to-Anion Proton Transfer Reactions: Effects of Charge State on the Structures of Protein Ions”

9:00 *Nicole D. Wagner and David H. Russell*, Department of Chemistry, Texas A&M University, College Station, TX  
“Defining Non-Covalent Ubiquitin Homodimer Interfacial Interactions through Comparisons with Covalently-Linked Diubiquitin”

9:25 *Helen Cooper*, School of Biosciences, University of Birmingham, Birmingham, UK  
“Differential ion mobility and top-down mass spectrometry for the analysis of proteins from complex biological samples”

9:50 *Coffee Break*  
*Victoria Ballroom*

**Proteins: Structure and Dynamics (Part 1)**

Chair: *Gary Glish*

10:20 *Brandon Ruotolo*, University of Michigan, Ann Arbor, MI  
“New Ion Mobility-Mass Spectrometry Techniques for the Rapid Analysis of Protein Sequence, Structure and Stability”

10:40 *Francisco Fernandez-Lima*, Florida International University  
“Advantages of TIMS-TOF MS and TIMS-FT-ICR MS for Complex Mixture Analysis and Structural Biology”

11:00 *Lekha Sleno*, Université du Québec à Montréal, Montréal, QC  
“Quantitation of acetaminophen protein binding in human plasma”

11:20 **Kristina Hakansson**, University of Michigan, Ann Arbor, MI  
*“Tandem Mass Spectrometry Approaches to the Elucidation of Sulfur-Associated Protein Modifications”*

11:40 **Christoph Borchers**, University of Victoria - Genome BC Proteomics Centre, Victoria, BC  
*“Solving Protein Structures by Cross Linking - Discrete Molecular Dynamics”*

12:00 Discussion and **Workshop group picture**

12:15 to 13:30 Lunch  
**Fairview Dining Room**

**Endogenous Peptides**      Chair: **Peter Verhaert**

14:00 Introductory Remarks: **Peter Verhaert**

14:05 **Lingjun Li**, University of Wisconsin, Madison, WI  
*“Enabling Large-Scale Discovery, Characterization and Quantitation of Neuropeptides via Tandem Mass Spectrometry”*

14:30 **Paul Thomas**, Northwestern University, Chicago, IL  
*“Top Down Proteomics in the Age of Proteoforms”*

14:55 **Geert Baggerman**, University of Antwerp, Antwerp, Belgium  
*“Micro peptides as a new class of bio-active peptides in higher eukaryotes”*

15:20 **Luuk van Oosten**, Heidelberg University, Heidelberg, Germany  
*“Tandem MS structure elucidation of disulfide containing peptides from ant venom after determining their S-engendered mass defect and isotope shift using high resolution MS”*  
**Lake Louise Student Travel Award Winner**

15:40 Coffee Break  
**Victoria Ballroom**

**Bio-Applications, Proteomics**      Chair: **David Schriemer**

16:10 **Daniel Lopez Ferrer**, Thermo Fisher Scientific, San Jose, CA  
*“Applications of UVPD for Top Down Proteomics on an Orbitrap Fusion Lumos Mass Spectrometer”*

16:30 **Arash Zarrine-Afsar**, University of Toronto, Toronto, ON  
*“Rapid Detection of Breast Cancer with an Optimized MS Analysis Workflow”*

16:50 **Dirk Valkenburg**, University of Georgia, VITO, Mol, Belgium  
*“PRiSM: A universal search engine for peptidomics and proteomics”*

17:10 **Anas El-Aneed**, University of Saskatchewan, Saskatoon, SK  
*“Mass spectrometric approaches to assess the cellular fate of lipid-based drug delivery systems”*

17:30 Discussion

18:00 Dinner

**Mount Temple Ballroom C**

**Gas Phase Ion Chemistry**

Chair: **Paul Mayer**

19:30 **Travis Fridgen**, Memorial University, St. John's, NL  
*“The structures of  $\text{Ca}^{2+}$  (Uracil)<sub>4-6</sub> and cationized aromatic half-belts”*

19:50 **Nicholas Riley** and Joshua Coon, University of Wisconsin, Madison, WI  
*“Activated Ion Electron Transfer Dissociation on an Orbitrap Fusion Mass Spectrometer”*  
**Winner of the Marg Northcott Lake Louise Student Travel Award**

20:10 **Ivan Chu**, University of Hong Kong, Hong Kong  
*“Radical-Mediated Peptide Tyrosine Nitration”*

20:30 **Sydney Wellman** and **Rebecca Jockusch**, University of Toronto, Toronto, ON  
*“Unravelling environmental effects: Photodissociation action spectroscopy and fluorescence of gaseous Chl a”*  
**NSERC CREATE Travel Award Winner**

20:50 **K. W. Michael Siu**, University of Windsor, Windsor, ON  
*“Gas-Phase Dehydration of Protonated Polyglycines”*

**21:10 Poster Session** (Authors are asked to be present until 23:00)

**Victoria Ballroom**

**Xuguang Liu** and Shawn Li, The University of Western Ontario, London,  
*“An AP-MS method for profiling tyrosine kinase activity in cancer”*

**John Sausen**, Agilent Technologies, Oconomowoc WI  
*“Integrating Highly Accurate Collision Cross Section Measurements into Metabolomic Screening and Discovery Workflows for Increased Identification and Detection Confidence”*

**Travis Falconer**, U.S. FDA, Cincinnati, OH  
*“HCD vs rCID for Qualitatively Significant Product Ions”*

**Annie von Eyken**, McGill University, Montreal, QC  
*“Development of a fast screening and quantification method of ten antimicrobials in honey using direct injection in HPLC-QTOF-MS/MS”*

**Christof Rampitsch**, Agriculture & Agrifood Canada, Morden, MB  
*"Mining the wheat leaf apoplast for effector proteins of Puccinia triticina"*

**Randy Purves**, University of Saskatchewan, Saskatoon, SK  
*"Semi Quantitative LC-SRM workflow for the analysis of over 100 polyphenols in lentil crops"*

**Jean Lodge**, Jessica Rabuck-Gibbons, Anna K Mapp, Brandon T. Ruotolo, University of Michigan Ann Arbor, MI  
*"Dissecting activator-coactivator interactions using collision induced unfolding"*

**Paul Mayer**, Department of Chemistry, University of Ottawa, Ottawa, ON  
*"Gas phase reaction dynamics of ionized PAHs"*

**Krishna Anapindi** and Jonathan V. Sweedler, University of Illinois, Urbana, IL  
*"Mass spectrometry based label-free quantitation of peptides involved in opioid-induced hyperalgesia"*

**Kevin A. Kovalchik**<sup>1</sup>, M.S. MacLennan<sup>1</sup>, Chukwuemeka Ajaero<sup>2</sup>, K.M. Peru<sup>3</sup>, D.W. McMartin<sup>2</sup>, J.V. Headley<sup>3</sup>, D.D.Y. Chen<sup>1</sup> <sup>1</sup>University of British Columbia, Department of Chemistry, Vancouver, BC., V6T 1Z1, <sup>2</sup>University of Regina, Faculty of Engineering and Applied Science, Regina, SK., S4S 0A2, <sup>3</sup>Environment and Climate Change Canada, Science and Technology Branch, Saskatoon, SK., S7N 3H5  
*"Characterization of Amine-Derivatized Naphthenic Acids by High Resolution Tandem Mass Spectrometry"*

**David Schriemer**, University of Calgary, Calgary, AB  
*"Neprosin-I as an alternative protease for middle-down proteomics"*

Bill Loyd, Robert E. Haufler, and **Doug Simmons**, SCIEX, Concord, ON  
*"N-Geometry TOF analyzer for ESI-QqTof"*

**Matthew F. Bush**, Samuel J. Allen, Rachel M. Eaton, Department of Chemistry, University of Washington, Seattle, WA  
*"Tandem Ion Mobility of Native-like Ions using Structures for Lossless Ion Manipulations"*

**Victor Yin** and Lars Konermann, The University of Western Ontario, London, ON  
*"Investigating the Effects of In situ Oxidation on the Structure and Non-Canonical Functions of Cytochrome C using Electrospray Mass Spectrometry"*

**Lars Konermann**, Tilo Schachel, Vlad Popa, The University of Western Ontario, London, ON  
*"Molecular Dynamics Simulations of Analyte Fragmentation in MS/MS: Bringing Together Theory and Experiment"*

**Dwain Cardona**, ThermoFisher, C. Postigo, C. Cojocariu, S.D. Richardson, Damia Barcelo, Per Nilsson  
*Use of Gas Chromatography Orbitrap Mass Spectrometry for small molecule discovery: iodinated disinfection byproducts as case study.*

## FRIDAY, DECEMBER 2

### Proteins: Structure and Dynamics (Part 2)

Chair: **Susan Richardson**

- 8:00 **Frank Sobott** University of Antwerp, Antwerp, Belgium  
*"Top-down and native ETD of proteins and complexes"*
- 8:20 **Derek J. Wilson**, York University, Toronto, ON  
*"Translating mass spectrometry enabled hydrogen deuterium exchange to drug development in neurodegenerative disease and cancer"*
- 8:40 **Haidy Metwally** and Lars Konermann, Department of Chemistry, The University of Western Ontario, London, ON  
*"Mechanism of protein supercharging by sulfolane and mNBA"*  
**Winner of a CSMS Travel Award, sponsored by Waters**
- 9:00 **Jason J. Serpa**; Evgeniy V. Petrotchenko; Christoph H. Borchers, UVic Genome BC Proteomics Centre, Victoria, BC  
*"Structure of prion  $\beta$ -oligomers as determined by structural proteomics"*  
**Winner of a CSMS Travel Award, sponsored by Thermo Fisher**
- 9:20 **Peter Tieleman** University of Calgary, Calgary, AB  
*"Computer simulations of membrane proteins"*
- 9:40 *Coffee Break*  
**Victoria Ballroom**

### Food, Environment, and other MS/MS Applications

Chair: **Gary Glish**

- 10:10 **Xing-Fang Li**, University of Alberta, Edmonton, AB  
*"Sweetened Swimming pools"*
- 10:30 **Susan Richardson**, University of South Carolina, Columbia, SC  
*"Hydrofracking Impacts on Drinking Water: High Resolution-MS and Tandem MS Uncovering New Chemical By-Products"*
- 10:50 **X. Chris Le**, University of Alberta, Edmonton, AB  
*"Mass spectrometry characterization of novel arsenic metabolites"*
- 11:10 **Stephane Bayen**, McGill University, Montreal, QC  
*"From targeted to non-targeted analysis: applications to food safety"*
- 11:30 **Brigitte Simons**, SCIEX, Concord, ON  
*"Turning new keys and making money; the demand for LC-MS iMETHODs"*
- 11:50 Discussion

12:15 to 13:30 Lunch

**Fairview Dining Room**

Friday Afternoon: Free time – Enjoy the Great Outdoors!

18:00 Cocktails

**Victoria Foyer / Victoria Ballroom**

19:00 Banquet

**Victoria Ballroom**

## SATURDAY, DECEMBER 3

### Health and Disease

Chair: **Lars Konermann**

8:10 **John McLean**, Vanderbilt University, Nashville, TN

*“Advances in Structural Mass Spectrometry for Metabolomics and Medicine”*

8:30 **Mona Hamada**, University of Saskatchewan, Saskatoon, SK

*“The development of novel targeted metabolomic methods for the diagnosis of respiratory illnesses”*

**Winner of a CSMS Travel Award, sponsored by Sciex**

8:50 **Mari DeMarco**, Providence Health Care & University of British Columbia, Vancouver, BC

*“Alzheimer disease biomarkers in patient care: A mass spec solution to a sticky situation”*

9:10 **Bingyun Sun**, Simon Fraser University, Burnaby, BC

*“Do biomarkers exist?”*

9:30 **Per Andrén**, Uppsala University, Uppsala, Sweden

*“Mass spectrometry imaging – opportunities for drug discovery and neuroscience”*

9:55 Coffee Break

**Victoria Ballroom**

### Saccharides, Lipids, Metabolites

Chair: **Peter Verhaert**

10:30 **Jon Amster** University of Georgia, Athens, GA

*“ Ion Mobility Studies of Glycosaminoglycan-Protein Complexes”*

10:50 **Pietro Morlacchi**, Agilent Technologies, Saint Laurent, QC

*“Mass Spectrometry as it relates to metabolomics and cell energetics studies”*

- 11:10 **Brian Clowers** Washington State University, Pullman, WA  
*“Frequency Encoded Mobility Separations and Fragmentation Yields for Isomeric Tetrasacharides”*
- 11:30 **Gary Glish** University of North Carolina, Chapel Hill, NC  
*“A Simple Mass Spectrometry Method to Identify Mono and Disaccharides”*
- 11:50 **Jeffrey Smith**, Carleton University, Ottawa, ON  
*“Recent improvements in TrEnDi chemistry: enhancing plasmalogen and sphingomyelin signal and allowing fatty acyl identification”*
- 12:10 Discussion and Adjournment
- 12:15 to 13:30 Lunch  
***Fairview Dining Room***

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The top category: “Double Black Diamond” is currently vacant.