

**LAKE LOUISE XXXII**  
**32<sup>nd</sup> Workshop on Tandem Mass Spectrometry**  
**REVISED 2019-12-01**

THURSDAY, DECEMBER 5

8:00 Introductory Remarks: **Lars Konermann**

**Allergens and Antibodies**

Chair: **Lars Konermann**

- 8:10 **Michael L. Gross**, Washington University in St. Louis  
*“Proteomics for Antibody/Antigen Structure and Interactions”*
- 8:35 **Lisa Marzilli**, Jeff Grassie, Elaine Stephens, Roger Theberge, Mellisa Ly, Leah Wang, Peilu Liu, Dennis Gessmann and Jason Rouse, Pfizer  
*“Enhancing Product Knowledge and Future Molecular Design by Elucidating and Cataloging CDR Sequence Instabilities in Monoclonal Antibodies”*
- 9:00 **Jens Brockmeyer**, Julia Brucker, Robin Korte, University Stuttgart  
*“Allergen detection and elucidation of the gastrointestinal allergen metabolism using LC-MS/MS”*
- 9:25 **Melanie Downs**, University of Nebraska-Lincoln  
*“Mass Spectrometry Methods for Food Allergen Analysis: Panacea or Pandora’s Box?”*

9:50 Coffee Break  
**Victoria Ballroom**

**Proteins and Peptides**

Chair: **Kicki Håkansson**

- 10:20 **Christopher Thibodeaux**, Yeganeh Habibi, Kevin Uggowitzer, Hassan Issak, McGill University  
*“Examining the Role of Conformational Changes in Natural Product Biosynthesis using Hydrogen-Deuterium Exchange Mass Spectrometry”*
- 10:40 **Roger Liu**, Mengru Zhang, Bojie Zhang, Don L. Rempel, Michael L. Gross, Washington University in St. Louis  
*“Hydroxyl-Radical Reaction Pathways for the Fast Photochemical Oxidation of Proteins Platform As Revealed by <sup>18</sup>O Isotopic Labeling”*  
**Marg Northcott Lake Louise Student Travel Award**
- 11:00 **Yehia Mechref**, Texas Tech University  
*“Analysis of Glycans and Glycopeptides by LC-MS/MS”*
- 11:20 **Ryan Julian**, University of California, Riverside  
*“Peptide isomer detection by RDD: Connecting Alzheimer’s disease and the lysosome”*

11:40 **Chad Weisbrod**, Lissa C. Anderson, Jeffrey Shabanowitz, Donald F. Hunt, Christopher L. Hendrickson, National High Magnetic Field Laboratory  
*“Advances in Proton Transfer Reactions and Parallel Ion Parking for Intact Protein Analysis on a 21 T FT-ICR Mass Spectrometer”*

12:00 **Workshop group picture**

12:15 to 13:30 Lunch

**Fairview Dining Room**

**Advances in Methods and Instrumentation I**

Chair: **Gary Glish**

14:00 **Christian Klein**, Agilent Technologies Inc.

*“Novel capabilities in gas phase separation and reaction on high resolution accurate mass instruments”*

14:25 **Steffen Lindert**, Ohio State University

*“Computational Protein Structure Prediction from Mass Spectrometry Data”*

14:45 **Charlie Schmidt**, PerkinElmer

*“Novel Applications using LCMSMS”*

15:05 **Richard Oleschuk**, Prashant Agrawal, Haidy Metwally, Kasia Donovan, Matthias Hermann, Ben Tucker, Tim Solamons, Queen's University

*“(Super)hydrophobic Surfaces for Mass Spectrometric Sample Preparation and Tissue Blotting/Imaging”*

15:25 **Jakub Ujma**, Kevin Giles, David Ropartz, Dale Cooper-Shepherd, Martin Palmer, Mike McCullagh Waters

*“Development and application of a cyclic ion mobility mass spectrometer”*

15:45 Coffee Break

**Victoria Ballroom**

**Environmental Chemistry**

Chair: **Jeff Smith**

16:15 **Chris Le**, Hanyong Peng, University of Alberta

*“Mass spectrometry for environmental research”*

16:35 **Susana Kimura-Hara**, Alejandro Ortega-Hernandez, Raphael Acabaya, University of Calgary

*“Wastewater Reuse in Canada: Priority Disinfection By-products in a Full-Scale Wastewater Reuse Facility”*

16:55 **Xing-Fang Li**, Caley Craven, University of Alberta

*“HPLC-MS/MS Evidence of 96 pesticides in cannabis growing environment, an ignored source of human exposure”*

17:15 **Susan Richardson**, University of South Carolina

*“Potential Impacts of Hydraulic Fracturing on Drinking Water: High-Resolution-Tandem Mass Spectrometry Identification of >300 Novel Surfactant-Derived S-DBPs”*

17:35 Discussion

18:00 Dinner

*Mount Temple Ballroom C*

**Proteomics**

Chair: *Peter Verhaert*

19:15 **Pierre Thibault**, Q. Zhao, J.-P. Laverdure, J.Lanoix, C. Durette, C. Cote, S. Pfammatter, E. Bonneil, C. M. Laumont, P. Gendron, K. Vincent, S. Lemieux, D. G. Millar, P. S. Ohashi, C. Perreault, Université de Montréal/ IRIC

*“Immunopeptidomic dark matter reveals unsuspected targets for cancer immunotherapy”*

**CSMS Fred Lossing Award**

19:40 **Felix Meissner**, Annika Frauenstein, Sebastian Vierreira Winter, Daniel Hornburg, Matthias Mann, Max Planck Institute of Biochemistry

*“Highly multiplexed absolute quantification of communicating immune cells with EASI-tag”*

20:00 **Trisha Tucholski**, Ying Ge, University of Wisconsin-Madison

*“Tandem MS Characterization of Large Proteoforms (up to 140 kDa) Enabled by Novel Top-down Proteomics Strategy”*

**Lake Louise Student Travel Award**

20:20 **Samaneh Dastpeyman**, Heng Jiang and Ann M. English, Concordia University

*“Proteomics analysis of yeast response to H<sub>2</sub>O<sub>2</sub> challenge on mutation of a H<sub>2</sub>O<sub>2</sub> sensor into a hyper sensor”*

**CSMS Travel Award, sponsored by Waters**

20:40 **Thomas Kislinger**, Princess Margaret Cancer Centre

*“Identification of Aggressive Prostate Cancers: In-depth Proteomics of Tissues and post-DRE Urines”*

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

*Victoria Ballroom*

**Darien Yeung**, Vic Spicer, Oleg Krokhin, Manitoba Centre of Proteomics and Systems Biology

*“Peptide retention time prediction for mixed-mode chromatographic separation in the first dimension of 2D LC-MS/MS for bottom-up proteomics”*

**Banafsheh Mehrazma**, Xiaojing Huang, Sladjana Slavkovic, Cristina Lento, Philip Johnson, Gary Sweeney, Derek J. Wilson, York University

*“The Peculiar Unfolding of Lipocalin 2 in the Presence of Siderophores”*

**Christof Rampitsch**, Agriculture & Agri-Food Canada

*“What are peptides contributing to the wheat-leaf rust interaction?”*

**Gaëlle Bridon**, Sheher Mohsin; Sanjib Meitei; Peter Siegel; Daina Avizonis, AGILENT

*“Fast Supercritical Fluid Chromatography Separation and Shotgun Lipidomics with High Resolution Mass Spectrometry for the Study of Breast Cancer Metastasis”*

**Kyle Brown**, Bifan Chen, Tania Guardado, Ziqing Lin, Song Jin, Ying Ge, University of Wisconsin-Madison

*“Online tandem MS characterization on membrane proteins enabled by a photocleavable surfactant”*

**Stephen Valentine**, Sandra Majuta, Sara Macios, West Virginia University

*“Hydrogen-deuterium exchange with tandem MS for isomer discrimination”*

**Rimanpreet Kaur**, Amit Prasad, IIT MANDI

*“Identification of proteins in the cyst fluid of Taenia solium by Tandam MS”*

**Marie-Christine Tang**, Hao Yang, Wei Peng, Shupeí Wang, Grant A. Mitchell, and Alexandra Furtos, Université de Montréal

*“Method development for quantitation of NTBC in mouse plasma and liver”*

**Louiza Mahrouche**, Alexandra Furtos, Guillaume Leonard, Serge Marchand, Université de Montréal

*“LC-MS/MS approach for four endocannabinoids quantitation in human plasma”*

**John Headley**, Environment and Climate Change Canada

*“Molecular characterization of oil sands naphthenic acids in natural wetlands”*

**Leanne Martin**, Lars Konermann, University of Western Ontario

*“Enhancing Protein Electrospray Charge States by Multivalent Metal Ions: Mechanistic Insights from MD Simulations and Mass Spectrometry Experiments”*

**Victor Yin**, University of Western Ontario

*“Delineating Metal-Catalyzed versus ?Bulk? Protein Oxidation Mechanisms in Cytochrome c: Are We Seeing the Big Picture?”*

**Nastaran Nosrat Tajoddin**, Lars Konermann, Western University of Ontario

*“Conformational Dynamics and Aggregation of Thermally Stressed Proteins Studied by Hydrogen/Deuterium Exchange Mass Spectrometry”*

**Elnaz Aliyari**, Lars Konermann, The University of Western Ontario

*“Investigating the Mechanism of Protein Electrospray Ionization”*

**Ying Chen**, Tao Huan, University of British Columbia

*“Global-Scale Profiling of Human Hair Metabolome and Exposome”*

**Alan de Aguiar Lopes**, Heng Jiang, Ann M. English, Concordia University

*“Proteomic analysis of yeast cells treated with the antifungal miconazole”*

**Andrew Michael**, David C Schriemer, University of Calgary

*“In vivo XL-MS facilitated by freeze substitution”*

**Mengru Zhang**, Brett R. Beno, Richard Y.-C. Huang, Jagat Adhikari, Ekaterina G. Deyanova, Jing Li, Guodong Chen, Michael L. Gross, Washington University in St Louis

*“An Integrated Approach to Afford Effective Binding Interface Determination of IL-7/IL-7R? In-solution and the Evaluation of HDX Kinetics Adjudicating Candidate Docking Models”*

**Bruno do Amaral**, Fabio C. Gozzo, University of Calgary

*“Acidic XPlex: a multiplex alternative to NHS esters for faster cross-linking reactions at low temperatures”*

**Michael Andersen**, Evosep

*“A Novel LC System Embeds Analytes in Pre-formed Gradients for Rapid, Ultra-Robust Proteomics”*

**Asmita Poudel**, George Gachumi, Ildiko Badea, Anas El-Aneed, University of Saskatchewan

*“Liquid Chromatography Tandem Mass Spectrometry (LC-MS/MS) Method for Simultaneous Quantification of Phytosterols and Tocopherols entrapped in Lipid based Nano-formulation”*

**Lars Konermann**, The University of Western Ontario

*“Protein Charging and Supercharging during ESI”*

## FRIDAY, DECEMBER 6

### Guns, Drugs, and Alcohol

Chair: *Jon Amster*

- 8:00 **Jack Henion**, Daniel Eikel and Changtong Hao, Advion, Inc.  
“*The Role of Mass Spectrometry in the Cannabis Industry*”
- 8:25 **Donald Land**, University of California, Davis  
“*Applications of Mass Spectrometry in Cannabis Regulatory Testing and Research*”
- 8:50 **Philippe Schmitt-Kopplin**, Helmholtz Zentrum Muenchen  
“*Ultrahigh resolution mass spectrometry in Foodomics: from fermented beverages to distillates*”
- 9:15 **Randall Clark**, Auburn University  
“*GC-MS and Product Ion MS/MS Studies on Synthetic Designer Drugs: Cannabinoids, Cathinones and N-BOMes*”
- 9:40 **Greg Gillen**, NIST  
“*Molecular Imaging Mass Spectrometry for Characterization of Explosives and Illicit Narcotics*”

10:05 *Coffee Break*  
*Victoria Ballroom*

### Drugs and Metabolites

Chair: *Susan Richardson*

- 10:35 **Jeffrey Smith**, Wondewossen Gebeyehu, Karl V. Wasslen, Robert Boyd, Lynne Leonard, Carleton University  
“*Rapid drug checking in a supervised injection site using portable mass spectrometry*”
- 10:55 **Robert Di Lorenzo**, Craig Butt, KC Hyland, Nour Mashmoushi, Scott Hopkins, Larry Campbell, Christopher Borton, SCIEX  
“*Know Your Grow: Phenotyping cannabis using mass spectrometry*”
- 11:15 **Wei Jin**, Mays Al-Dulaymi, Randy Purves, Ildiko Badea, Ed Krol and Anas El-Aneed, University of Saskatchewan  
“*Mass spectrometric investigation on the biological fate of gemini surfactants used as gene delivery vectors*”  
**CSMS Travel Award sponsored by Thermo Fisher Scientific**
- 11:35 **Erica Forsberg**, Asha Goodman, Robert A. Edwards, San Diego State University  
“*Development of a shark health matrix using metabolomics coupled with metagenomics*”
- 11:55 **Tao Huan**, University of British Columbia  
“*Global Metabolomics and Systems Biology*”
- 12:15 **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 7

### Metabolites, Glycans, Ion Chemistry

Chair: **Lars Konermann**

8:00 **Jon Amster**, University of Georgia

*“Capillary Zone Electrophoresis and Tandem Mass Spectrometry for the Analysis of Glycosaminoglycans”*

8:20 **Calvin Chan**, Jiaxi Peng, Julian Lamanna, Aaron R. Wheeler, University of Toronto

*“Targeted Laser Cell Lysis on Digital Microfluidics for Single-cell Proteomics”*

**NSERC CREATE Travel Award**

8:40 **Paul Mayer**, Brandi J. West, Malick Diedhiou, Maxi Burgos-Paci, Christine Joblin, University of Ottawa

*“Ion Chemistry from the Atmosphere to Interstellar Space”*

9:00 **Neville Coughlan**, Patrick J. J. Carr, Stephen C. Walker, Ce Zhou, Mircea Guna, J. Larry Campbell, & W. Scott Hopkins, University of Waterloo

*“A tandem DMS-MS experiment for spectroscopic interrogation of molecular ions”*

**CSMS Travel Award sponsored by Sciex**

9:20 **Kristina Hakansson**, Hye Kyong Kweon, Isaac Agyekum, Andy T. Kon, Shijiao Huang, Alexey I. Nesvizhskii, Yanzhuang Wang, Philip C. Andrews, University of Michigan

*“Novel Approaches to the MS/MS Analysis of Sulfated Molecules”*

9:40 Coffee Break

**Victoria Ballroom**

## **Advances in Methods and Instrumentation II**

Chair: *David Schriemer*

- 10:10 **Derek Wilson**, Cristina Lento, Shenbaga Moorthy, Banafsheh Mehrazma, York University  
*“Illuminating the 'dark' phase of amyloidogenesis in anti-neurodegenerative drug development”*
- 10:30 **Ken Miller**, Thermo Fisher  
*“High Throughput Single Cell Proteome Analysis with Nanodroplet Sample Processing, Multiplex TMT Labeling, and Ultra-Sensitive LC-MS”*
- 10:50 **Francisco Fernandez-Lima**, Florida International University  
*“Recent Advances in TIMS-MS”*
- 11:10 **Ann English**, Soran Jahangiri, Heng Jiang, Qadir Timerghazin and Gilles H. Peslherbe  
Centre for Biological Applications of Mass Spectrometry (CBAMS) and Centre for Research in  
Molecular Modelling (CERMM), Concordia University, Montreal.  
*“Computational Insights into the Mass Spectra of TEMPOM<sup>+</sup> ions”*
- 11:30 **Gary Glish**, Tiffany Crawford, Matthew Campbell, University of North Carolina  
*“What is coming out of your ESI source might not be what you think”*
- 11:50 **Peter Verhaert**, ProteoFormiX BV  
*“Towards the identification of novel disease biomarkers by tandem MS directly from patient tissue”*
- 12:10 Discussion and Adjournment

12:15 to 13:30 Lunch

***Fairview Dining Room***

We gratefully acknowledge financial support for the Lake Louise Workshop

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