

# LAKE LOUISE XXXI

## 31<sup>st</sup> Workshop on Tandem Mass Spectrometry

THURSDAY, NOVEMBER 29

8:00 Introductory Remarks: *Lars Konermann*

### Metabolomics 1                      Chair: *Peter Verhaert*

8:10 *Ron Heeren*, Maastricht University, Maastricht, The Netherlands  
“High throughput tandem Imaging MS in personalized medicine”

8:35 *Jing Fan*, and *Gretchen Seim*, *Emily Britt*, *Aaron Johnson*, Morgridge Institute / University of Wisconsin-Madison, Madison, USA  
“Understanding dynamic metabolic rewiring in macrophages using metabolomics”

9:00 *Philip Britz-McKibbin*, McMaster University, Hamilton, ON, Canada  
“Multiplexed Separations for Biomarker Discovery in MS-based Metabolomics: Boosting Throughput and Data Fidelity with Quality Assurance”

9:25 *Dietrich Volmer*, Humboldt University, Berlin, Germany  
“Vitamin D Metabolism and Clinical Metabolic Phenotyping”

9:50 *Coffee Break*  
*Victoria Ballroom*

### Peptides and Proteins 1                      Chair: *Jon Amster*

10:20 *Helen Cooper*, University of Birmingham, Birmingham, UK  
“LESA mass spectrometry for top-down protein analysis of microbes”

10:40 *Christopher Thibodeaux*, McGill University, Montreal, QC, Canada  
“Exploring Frontiers in Natural Product Peptide Biosynthesis with Mass Spectrometry”

11:00 *K. W. Michael Siu*<sup>2</sup>, *K.H. Brian Lam*<sup>1</sup>, *Justin Kai-Chi Lau*<sup>1,2</sup>, *Cheuk-Kuen Lai*<sup>1</sup>, *Alan C. Hopkinson*<sup>1</sup>  
<sup>1</sup>Department of Chemistry and Centre for Research in Mass Spectrometry, York University; and  
<sup>2</sup>Department of Chemistry and Biochemistry, University of Windsor University of Windsor, Windsor, ON, Canada  
“Structures and Fragmentation of the  $[b_n]^+$  Ions from Dehydration of Polyglycines”

11:20 *Ivan Chu*, The University of Hong Kong, Hong Kong, China  
“Formation, Isomerization and Dissociation of Peptide Radical Cations: Structural, Mechanistic, and Photodissociation Spectroscopic Investigations”

11:40 *Neena Susan Eappen* and *Rebecca Jockusch*, University of Toronto, Toronto, ON, Canada  
“Structural characterization of peptides using gas phase Hydrogen Deuterium Exchange”  
**Winner of the NSERC CREATE Travel Award**

12:00 **Workshop group picture**

12:15 to 13:30 Lunch

**Fairview Dining Room**

**Peptides and Proteins 2**

Chair: **Lars Konermann**

14:00 **Sibylle Pfammatter**<sup>1, 2</sup>, **Eric Bonneil**<sup>1</sup>, and **Pierre Thibault**<sup>2</sup>, <sup>1</sup>Institute for Research in Immunology and Cancer, University of Montreal, Montreal, QC; <sup>2</sup>Department of Chemistry, University of Montreal, Montreal, QC; <sup>3</sup>Univ.of Montreal, Montreal, QC, Canada

*“Impact of high field asymmetric waveform ion mobility spectrometry (FAIMS) on quantitative proteomics and the profiling of protein modifications”*

**Winner of the Marg Northcott Lake Louise Student Travel Award**

14:20 **Derek J. Wilson**, **Cristina Lento** and **Ruth Knox**, York University, Toronto, ON, Canada

*“Linking Specific Dynamic Modes to the Catalytic Reaction Coordinate in Enzymes via Millisecond H/D Exchange”*

14:40 **Alan Kadek**, **Knut Koelbel**, **Kristina Lorenzen**, **Jens Buck** and **Charlotte Uetrecht**, Heinrich Pette Institute / European XFEL, Hamburg, Germany

*“Hitting proteins with a sledgehammer - combining native MS with soft X-rays”*

15:00 **Thomas Kislinger**, Princess Margaret Cancer Centre, Toronto, ON, Canada

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

15:20 **John McLean**, Vanderbilt University, Nashville, TN, USA

*“High dimensional molecular phenomics in systems, synthetic, and chemical biology”*

15:40 Coffee Break

**Victoria Ballroom**

**Environmental Chemistry**

Chair: **Lekha Sleno**

16:10 **Hannah K. Liberatore**, **M. J. Plewa**, **E. D. Wagner**, **J. M. Allen**, **A. A. Cuthbertson**, **D. C. Westerman**, **J. M. VanBriesen**, **D. B. Burnett**, **L. H. Cizmas**, **S. D. Richardson**, University of South Carolina, Columbia, SC, USA

*“Tandem MS and Impacts of Hydraulic Fracturing on Drinking Water: Important Ramifications for Human Health”*

**Winner of a Lake Louise Student Travel Award**

16:30 **Chenxing (Angela) Sun** and **Jonathan W. Martin**, University of Alberta, Edmonton, AB, Canada

*“Development and Application of Nontarget Mass Spectrometry Analysis of Organic Compounds in Hydraulic Fracturing Flowback and Produced Water”*

**Winner of a CSMS Travel Award sponsored by Thermo Fisher Scientific**

- 16:50 **TBA**, PerkinElmer  
*“Overcoming the Challenges Associated with Pesticide Analysis of Cannabis using a Dual Source LC-MS/MS”*
- 17:10 **Susan Richardson**, Kristin H. Cochran, Cassiana Montagner, Danielle Westerman, Dion D. Dionysiou, Ying Huang, Daniel Schlenk, and Keith Loftin, University of South Carolina, Columbia, SC, USA  
*“Turning Wastewater into Drinking Water: Non-target Identification of Treatment Products Using High Resolution and Tandem Mass Spectrometry”*
- 17:30 Discussion

18:00 Dinner  
**Mount Temple Ballroom A**

**Protein Covalent Modifications**

Chair: **Gary Glish**

- 19:30 **Ann English**, Concordia University, Montréal, QC, Canada  
*“New Insights into redox biology from proteoform profiling by LC-MS/MS”*  
**Winner of the CSMS Fred Lossing Award**
- 19:55 **Timon Geib**, and Lekha Sleno, Université du Québec à Montréal, Montreal QC, Canada  
*“HRMS/MS vs. MRM: Screening Protein Adducts of Acetaminophen and Clozapine”*  
**Winner of a CSMS Travel Award sponsored by Sciex**
- 20:15 **Guy Poirier**, Jean-Philippe Gagné and John M. Pascal, Laval University, Québec, QC, Canada  
*“Novel approaches to study covalent ADP-ribosylation by tandem mass spectrometry”*
- 20:35 **Daniel Ziemianowicz** and David Schriemer, University of Calgary, Calgary, AB, Canada  
*“Protein painting with photochemistry: increasing information content from carbene covalent labeling”*

**20:55 Poster Session** (Authors are asked to be present until 23:00)  
**Victoria Ballroom**

- Victor Yin**, Saeef Mian and Lars Konermann, Department of Chemistry, University of Western Ontario, London, ON, Canada  
*“Lysine Carbonylation is a Key Component During Chloramine-T-induced Peroxidase Activation of Cytochrome c”*
- Eduardo De La Toba**, Krishna D. B. Anapindi, Emily Grace Tillmaand, Ashley Lenhart, Jeff Guo, Qin Liu, and Jonathan V. Sweedler, University of Illinois at Urbana-Champaign, MI, USA  
*“Label-Free Mass Spectrometric Analysis of Peptides in Chronic Itch”*
- Marcus Kim**, Agilent Technologies, Mississauga, ON, Canada  
*“Separation and Quantitation of Seven Cannabinoids Using Supercritical Fluid Chromatography-Tandem Mass Spectrometry (SFC-MS/MS)”*
- Oleg Krokhin**, University of Manitoba, Winnipeg, MB, Canada  
*“Peptide separation orthogonality in 2D LC-MS/MS for bottom-up proteomics”*

**Ian Webb**, Indiana University Purdue University Indianapolis, Indianapolis, MN, USA  
*“Pseudo-MS4 on a Tandem Ion Mobility/Time-of-Flight for Gas-Phase Covalent Modification”*

**Christoph Rampitsch**, Agriculture & Agri-Food Canada, Morden, MB, Canada  
*“TBA”*

**Ethan Yang, Chiara Gamberi and Pierre Chaurand**, Université de Montréal, Montreal, QC, Canada  
*“Mapping the Fly Malpighian Tubule Lipidome by Imaging Mass Spectrometry”*

**Katherine Cordova**, Canadian Grain Commission, Winnipeg, MB, Canada  
*“Proteomic Profiling of Canadian Malting Barley and Wort”*

**Michelle Ting, Lars Yunker, Katie Hatlelid, Scott McIndoe**, University of Victoria, BC, Canada  
*“Monitoring Complex Reaction in Real Time using Tandem Mass Spectrometric Methods”*

**Lars Konermann, Haidy Metwally, Quentin Duez**, Department of Chemistry, The University of Western Ontario, London, ON, Canada  
*“Forming Gaseous Ions from Solution-Phase Proteins: The Mechanism of Electrospray Ionization”*

**Tao Fan and V.J. Barthelet**, Grain Research Laboratory, Canadian Grain Commission, Winnipeg, MB, Canada  
*“Development of GC/MS Methods for the Quantification of Cyanogenic Glycoside in Breads with Flaxseed”*

## FRIDAY, NOVEMBER 30

### Ion Activation

Chair: *David Schriemer*

- 8:00 **Kristina Hakansson**, Isaac Agyekum, Hye Kyong Kweon, University of Michigan, Ann Arbor, MI, USA  
*“Negative ion electron capture dissociation: novel applications and a new mechanism”*
- 8:20 **Vicki Wysocki**, Ohio State University, Columbus, OH, USA  
*“Surface-Induced Dissociation of Protein Complexes”*
- 8:45 **Chad Weisbrod**, Lissa C. Anderson, Donald F. Smith, Steve Beu, Greg Blakney, Christopher L. Hendrickson, National High Magnetic Field Laboratory, Tallahassee, FL, USA  
*“Novel Ion Manipulation and Activation for High-Field Fourier Transform Ion Cyclotron Resonance MS/MS”*
- 9:10 **Glen Jackson**, Zachary Sasiene, Praneeth Mendis, West Virginia University, Morgantown, WV, USA  
*“Charge Transfer Dissociation (CTD) Mass Spectrometry of Glycans”*
- 9:35 **Stephen Blanksby**, Queensland University of Technology, Brisbane, Australia  
*“Tandem mass spectrometry of lipids: elucidating the chemistry and mobility of big fat ions in the gas phase”*

10:00 Coffee Break  
*Victoria Ballroom*

### Lipids and Glycans

Chair: *Kristina Hakansson*

- 10:30 **Sam Shields** and **Jeff Smith**, Carleton University, Ottawa, ON, Canada  
*“Safe and Modular Introduction of Gaseous Diazoalkanes for Alkylation Enhancement of Glycerophospholipids for Analysis via LCMS and MS/MS”*  
**Winner of a CSMS Travel Award, sponsored by Waters**
- 10:50 **Jeff Manthorpe**, Carleton University, Ottawa, ON, Canada  
*“Trimethylation Enhancement using Diazomethane (TrEnDi). Past, Present, and Future from an Organic Chemist's Perspective”*
- 11:10 **Dajana Vuckovic**, Aliaksandr Naplyau, Cian Monnin, Nathaly Reyes Garces, Mariola Olkowicz, Sofia Lendor, Ezel Boyaci, Barbara Bojko, Janusz Pawliszyn, German Gomez-Rios, Concordia University, Montreal, QC, Canada  
*“In vivo solid-phase microextraction for lipidomics of brain”*
- 11:30 **Jon Amster**, University of Georgia, Athens, GA, USA  
*“CE-MS/MS of Glycosaminoglycans”*
- 11:50 **Mandy Bowman**, ThermoFisher  
*“Novel Approaches for Improved Small Molecule Identification and Characterization using Orbitrap ID-X Tribrid Mass Spectrometer”*

12:10 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 1

### Novel Methods and Instrumentation

Chair: **Lars Konermann**

8:20 **Gary Glish**, and **James E. Keating**, University of North Carolina, Chapel Hill, NC, USA  
*“Dual-nESI DIMS/MS/MS for Lipidomics”*

8:40 **David H. Russell**, **Michael Poltash**, **Jacob McCabe**, Texas A&M University, College Station, TX, USA  
*“A next-generation Native Ion Mobility-Mass Spectrometer”*

9:00 **Scott McIndoe**, University of Victoria, BC, Canada  
*“Real time analysis of reactions”*

9:20 **Francisco Fernandez-Lima**, Florida International University, Miami, FL, USA  
*“TIMS-MS: new developments for structural biology”*

9:40 **Carl Myerholtz**, Agilent Technologies, Santa Clara, CA, USA  
*“TBA”*

10:00 Coffee Break  
**Victoria Ballroom**

### Metabolomics 2

Chair: **Susan Richardson**

10:30 **Erica Forsberg**, San Diego State University, San Diego, CA, USA  
*“Microbiome Metabolomics and the Gut-Brain Axis”*

10:50 **Tao Huan**, **Amelia Palermo**; **Gary Siuzdak**, The University of British Columbia, Vancouver, BC, Canada  
*“Analysis of Archived Metabolomics Data to Identify Active Metabolites and Pathways”*

11:10 **Scott Hopkins**, University of Waterloo, Waterloo, ON, Canada  
*“Analyzing Humulone Content in Beer with Differential Mobility Spectrometry”*

11:30 **Robert Proos**, Sciex

*“Novel Scanning Tools for Simultaneous Quantitative and Qualitative Untargeted Metabolomics Workflow”*

11:50 **Lekha Sleno**, Amal Guesmi, Ons Ousji, Leanne Ohlund, Université du Québec à Montréal, Montreal QC, Canada

*“Metabolic activation of sunscreens and BPA analogs studied by LC-HRMS/MS”*

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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**\*Sponsorship levels correspond to the difficulty ratings of the Lake Louise downhill ski runs.  
The top category: “Double Black Diamond” is currently unoccupied.**