

# LAKE LOUISE XXX

## 30th Workshop on Tandem Mass Spectrometry

THURSDAY, NOVEMBER 30

8:00 Introductory Remarks: *Lars Konermann*

### Gaseous Biomolecular Ions: Theory and Experiment

Chair: *Lars Konermann*

8:10 *Scott Hopkins*, University of Waterloo, Waterloo, ON  
“Gas Phase Drug Discovery: Physicochemical Property Measurements with Differential Mobility Spectrometry”

8:35 *Nicolas C. Polfer*, University of Florida, Gainesville, FL  
“Multiplexing infrared photodissociation spectroscopy in a cryogenic trap”

9:00 *Ryan P. Steele*, University of Utah, Salt Lake City, UT  
“Probing ion structure with new quantum simulations”

9:25 *Stephen J. Valentine*, West Virginia University, Morgantown, WV  
“Hydrogen/Deuterium Exchange with Ion Mobility-Tandem MS for Ion Structure Characterization”

9:50 *Coffee Break*  
*Victoria Ballroom*

### Ion Dissociation Techniques and Instrumentation

Chair: *Gary Glish*

10:20 *Dustin Klein and Jennifer Brodbelt*, The University of Texas at Austin, Austin, TX  
“Structural characterization of GAGs using 193 nm and 213 nm UVPD”  
**Winner of the Marg Northcott Lake Louise Student Travel Award**

10:40 *Darien Yeung* and Scott McIndoe, University of Victoria, Victoria, BC  
“Energy-dependent Electrospray Ionization: A tool for determining molecular fragmentation”

11:00 *Jonathan Amster*, University of Georgia, Athens, GA  
“Quadrupolar Detection in FT-ICR Provides Mass Accuracy Independent from Ion Intensity”

11:20 *Michael Poltash and David Russell*, Texas A&M University, College Station, TX  
“Development of a High Resolution Ion Mobility Orbitrap Mass Spectrometer for the Investigation of Lipid Binding to the Ammonia Channel (AmtB)”

11:40 *Kicki Hakansson*, University of Michigan, Ann Arbor, MS  
“Radical-Driven Biomolecular MS/MS at both Polarities”

12:00 **Workshop group picture**

12:15 to 13:30 Lunch

**Fairview Dining Room**

**Proteomics – Part 1**

Chair: **Kicki Hakansson**

- 14:00 **Peter Verhaert**, ProteoFormiX, Beerse, Belgium  
*“Top-Down Proteomics on Formalin-fixed Paraffin-embedded Tissues - Making Biobanked Clinical Material accessible for Biomarker Discovery”*
- 14:20 **Shen Zhang and Anne-Claude Gingras**, The Lunenfeld-Tanenbaum Research Institute, Toronto, ON  
*“Revealing the DPP4 proteome: Discovery of novel substrates using N-terminal proteomics”*  
**Winner of a CSMS Travel Award sponsored by Sciex**
- 14:40 **Philip L. Loziuk**, Thermo Fisher Scientific  
*“Pushing the leading edge in protein quantitation: Integrated, precise, and reproducible proteomic workflows”*
- 15:00 **Felix Leung and Vathany Kulasingam**, University of Toronto, Toronto, ON  
*“A biomarker discovery platform for non-serous ovarian cancers using integrative proteomics”*  
**Winner of a CSMS Travel Award sponsored by Thermo Fisher Scientific**
- 15:20 **Alan Doucette**, Dalhousie University, Halifax, NS  
*“Detergent-based platforms for top down proteomics”*

15:40 Coffee Break

**Victoria Ballroom**

**Plant Metabolites and Drugs**

Chair: **Jeff Smith**

- 16:10 **Gianluca Giorgi**, University of Siena, Siena, Italy  
*“Metabolic fingerprinting of plants and wines”*
- 16:30 **Randall Purves**, University of Saskatchewan, Saskatoon, SK  
*“Rapid analysis of medically relevant compounds in faba bean seeds using tandem mass spectrometry”*
- 16:50 **Chris Gill**, Vancouver Island University, Nanaimo, BC  
*“Direct Mass Spectrometry Advances and Applications: Fast Membranes, Fentanyl and Other Trace Measurements”*
- 17:10 **Brigitte Simons**, SCIEX, Richmond Hill, ON  
*“LC-MS demand for the Cannabis Industry”*
- 17:30 Discussion

18:00 Dinner  
**Mount Temple Ballroom**

**Proteins**

Chair: **Jon Amster**

- 19:30 **Hélène Perreault**, University of Manitoba, Winnipeg, MB  
*“Quantitative analysis of IgG subclasses by MS”*  
**Winner of the CSMS Fred Lossing Award**
- 19:55 **Francisco Fernandez-Lima**, Florida International University, Miami, FL  
*“Application of native nESI-TIMS-MS for screening and structural biology”*
- 20:15 **Jackie Mosely**, Durham University, Durham, UK  
*“Protein interactions with lanthanide metal-ligand probes”*
- 20:35 **Kerene Brown and Derek Wilson**, York University, Toronto, ON  
*“Detailed Comparison of Innovator and Biosimilar Therapeutic Antibodies Using Native MS”*  
**Winner of the NSERC CREATE Travel Award**

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

**John V. Headley**, Watershed Hydrology and Ecology Research Division  
*MS/MS Evidence for steroidal naphthenic acids in oil sands process-affected water*

Mark P. Barrow<sup>1\*</sup>, Kerry M. Peru<sup>2</sup>, Matthias Witt<sup>3</sup>, Dena W. McMartin<sup>4</sup> and John V. Headley<sup>2</sup>  
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\*Corresponding author (M.P.Barrow@warwick.ac.uk, Tel: +44 (0) 24 76151013)

**Guenther Kahlert**, Institute for Systems Biology  
*Unbiased drug interaction using comprehensive quantitative SWATH-MS*

**Haidy Metwally**, University of Western Ontario  
*Molecular Dynamics Simulations of the Electrospray Process: Effects of 18-crown-6 on Protein Supercharging*

**Charlie Schmidt**, PerkinElmer  
*Reduction of Matrix interferences in Pesticide analysis of Cannabis*

**Peter Tieleman**, University of Calgary  
*Lipid-protein interactions are unique fingerprints for membrane proteins*

**Haixia Zhang**, University of Saskatchewan

*Optimization of folate extraction from pulse crop seeds and quantification using liquid chromatography mass spectrometry*

**Fatma Elzahraa Elessawy**, University of Saskatchewan

*Quantification of polyphenols in four cultivars of faba beans using LC-MS/MS*

**Yiming Xiao**, University of Western Ontario

*Mass Spectrometry Insights into Bone Remodeling: Probing Ligand Interaction of OPG Monomers and Dimers by H/D Exchange MS*

**Kang Jiang**, University of Saskatchewan

*Establishment of universal tandem mass spectrometric fingerprint of phytosterols in canola oil deodorization distillate with atmospheric pressure chemical ionization (APCI)*

**George Gachumi**, University of Saskatchewan

*Development of Liquid Chromatography- Atmospheric Pressure Chemical Ionization-Tandem Mass Spectrometry (LC-APCI-MS/MS) Method for the Simultaneous Determination of Phytosterols and Tocopherols Extracted from Canola Oil Deodorizer Distillate*

**David Schriemer**, Shaunak Raval, Vlad Sarpe, Depts. Of Chemistry and Biochemistry and Molecular Biology, University of Calgary

*Evaluating the automated detection of EX1 and EX2 exchange states in Mass Spec Studio 2.0*

**Christof Rampitsch**, Slavica Djuric-Ciganovic; Mei Huang, Agriculture & Agri-Food Canada

*The Apoplastic proteome of rust-resistant wheat reveals early responses to infection by Puccinia triticina*

**Pierangela Palma**, University of Urbino

*Analysis of selected OCPs in soil matrix with a new Liquid-EI UHPLC-MS/MS interface.*

**Yves Le Blanc**, SCIEX

*Mitigating fragmentation of peptides with controlled clustering*

**Deema Qasrawi**, University of Calgary

*Tandem mass spectrometric measurement of seven steroids in dried blood spots to diagnose congenital adrenal hyperplasia*

**Marcus Kim**, Agilent; Theresa Sosienski; Dan-Hui Dorothy Yang; Joan Stevens; Christian Heggmanns

*Analysis of Mycotoxins in Food Matrices using the Innovative Ultivo Triple Quad LC/MS*

**Daniel Beach**, National Research Council of Canada

*Tandem Mass Spectrometry Methods and Reference Materials for Tetrodotoxin Analysis*

**Victor Yin**, University of Western Ontario

*A Critical Examination of Oxidative Modifications: A Combined Bottom-up and Top-down Approach*

## FRIDAY, DECEMBER 1

### Proteomics – Part 2

Chair: **David Schriemer**

- 8:00 **Ray Bacala**, Grain Research Laboratory, Winnipeg, MB  
*“Investigation and analysis of Canadian wheat gluten in proteins”*
- 8:20 **Geert Baggerman**, VITO, Mol, Belgium  
*“Search for micropeptides, a new class of bioactive peptides”*
- 8:40 **Guy Poirier**, Laval University, Quebec City, QC  
*“Novel mass spectrometry method to identify PARP-1 substrates and interactors in cancer cells: improvement of PARP-1 inhibitor therapy”*
- 9:00 **Brandi West**, University of Ottawa, Ottawa, ON  
*“Direct observation of two component fibril assemblies through MALDI imaging”*
- 9:20 **Sibylle Pfammatter**, IRIC - Université de Montréal, Montréal, QC  
*“Ion mining through sample complexity? Impact of ion mobility on precision and depth of proteomic analyses”*
- 9:40 *Coffee Break*  
**Victoria Ballroom**

### Bio-Applications

Chair: **Peter Verhaert**

- 10:10 **Christoph Borchers**, University of Victoria - Genome BC Proteomics Centre, Victoria, BC  
*“Update on crosslinking based Structural Proteomics - from determining the structure of single proteins to analyzing organelle-wide protein-protein interactions”*
- 10:30 **Guenter Allmaier**, Vienna University of Technology (TU Wien), Vienna, Austria  
*“Nano ES-Differential Mobility Analysis (GEMMA) and mass spectrometry of intact viruses and liposomes”*
- 10:50 **Dirk Valkenburg**, Hasselt University, Diepenbeek, Belgium  
*“InSourcerer: a high-throughput method to search for unknown metabolite modifications by mass spectrometry”*
- 11:10 **Shane Tichy**, Agilent, Santa Clara, CA  
*“Redefining the Tandem Quadrupole Mass Spectrometer”*
- 11:30 **Davide Corinti and Simonetta Fornarini**, Università degli Studi di Roma “La Sapienza”, Rome, Italy  
*“MS coupled with IRMPD spectroscopy and fixed-wavelength kinetics to disclose isomeric mixtures of antitumor Pt(II)-complexes with amino acids”*  
**Winner of a Lake Louise Student Travel Award**
- 11:50 **Jeff Smith**, Carleton University, Ottawa, ON  
*“Recent Improvements in TrEnDi: Lipid Scope and Signal Consolidation”*

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 2

### Environmental Applications – Part 1

Chair: **Lars Konermann**

8:00 **Susan Richardson**, University of South Carolina, Columbia, SC

*“Can we make drinking water safer? Tandem mass spectrometry and a giant Brita filter”*

8:20 **Xing-Fang Li**, University of Alberta, Edmonton, AB

*“Halogenated peptides in drinking water”*

8:40 **Scott Mabury**, University of Toronto, Toronto, ON

*“Fascination with OrganoFluorine”*

9:05 **Achille Cappiello**, University of Urbino, Italy

*“LEI: a new, multipurpose LC-MS interface”*

9:30 **Janusz Pawliszyn**, University of Waterloo, Waterloo, ON

*“Direct coupling of sample preparation to mass spectrometry for rapid screening”*

9:55 Coffee Break

**Victoria Ballroom**

### Environmental Applications – Part 2

Chair: **Susan Richardson**

10:25 **Ping Jiang and Xing-Fang Li**, University of Alberta, Edmonton, AB

*“Identification of Organic Halogenated-Nitrogenous Disinfection Byproducts by Electrospray Tandem Mass Spectrometry”*

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

10:45 **Pierre Dumas**, Normand Fleury, Pierre Ayotte, Centre de Toxicologie du Québec, Québec, QC  
" Atmospheric pressure ionisation for gas chromatography (APGC) coupled to tandem mass spectrometry: New perspectives for the determination PCDD/F and "dioxin like PCB in human serum "

11:05 **Justin Renaud**, Agriculture and Agri-Food Canada, London, ON  
"Spectral Counting Approach to Measure Selectivity of High-Resolution LC/MS Methods"

11:25 **Chris Le**, University of Alberta, Edmonton, AB  
"Recent studies of arsenic speciation"

11:45 **Gary Glish**, University of North Carolina, Chapel Hill, NC  
"What's in that e-cigarette liquid?"

12:05 Discussion and Adjournment

12:15 to 13:30 Lunch

**Fairview Dining Room**

**Delegates staying over to Sunday, we have a special treat:**

18:00 to 22:00 Cocktails followed by a Christmas Dinner

**Victoria Ballroom**

We gratefully acknowledge financial support for the Lake Louise Workshop\*

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