

LAKE LOUISE XXVIII

28th Workshop on Tandem Mass Spectrometry

THURSDAY, DECEMBER 3

8:00 Introductory Remarks: *Lars Konermann*

Computational Methods for MS/MS Chair: *David Schriemer*

8:10 *Michael MacCoss*, University of Washington
“Building an Ecosystem of Software Tools for the Refinement, Application, and Dissemination of Methods for Targeted Peptide Quantitation”

8:35 *Dirk Valkenburg*, VITO
“CONSTAND: A method to eliminate systematic bias from labeled tandem MS data for quantitative proteomics”

9:00 *Shuzhao Li*, Emory School of Medicine
“Network prediction and data integration for systems medicine”

9:25 *Peter Horvatovich*, University of Groningen
“Proteogenomics approach to reveal the molecular changes in COPD patients”

9:50 Discussion and Coffee Break
Victoria Ballroom – Red Room

Structural Mass Spectrometry Chair: *Gary Glish*

10:20 *Derek Wilson*, York University
“Conformational Dynamics in Enzyme Catalysis and Ligand Binding”

10:40 *David Schriemer*, University of Calgary
“Tackling the n -squared problem in XL-MS”

11:00 *Christoph Borchers*, UVic Genome BC Protein Centre
“Towards solving protein structures by structural proteomics”

11:20 *John A. McLean*, Vanderbilt University
“Structural mass spectrometry for unraveling complex biology”

11:40 *Peter Tieleman* University of Calgary
“Lipid-protein interactions from combined experiments and simulation”

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

12:15 Lunch
Fairview Dining Room

Novel Methods and Instrumentation

Chair: *Kristina Håkansson*

- 14:00 **John Fjeldsted** Agilent Technologies
“Developments and Applications of Low Field Drift Ion Mobility - Mass Spectrometry”
- 14:20 **Alejandro Cohen**, Dalhousie University
“The Antidote to Nano-LC's Achilles' heel: Real-time Post-Column Flowrate measurements of nano-LC eluent by Digital Image Analysis”
- 14:40 **Oleg Krokhin**, Peyman Ezzati, Vic Spicer, John A. Wilkins University of Manitoba
“3D LC-MS/MS of whole cell lysate digests: deep proteome coverage and accurate retention data collection”
- 15:00 **K. W. Michael Siu**, University of Windsor
“Proposed Nomenclature for Peptide ion fragmentation”
- 15:20 **Christopher A. Wootton**, Peter O'Connor, University of Warwick
“Studying the effects of metal complexes in ultra-high resolution FT-ICR tandem mass spectrometry of metal-bound biomolecules”
Lake Louise Student Travel Award
- 15:40 Discussion and Coffee Break
Victoria Ballroom – Red Room

Glycochemistry and Glycobiology

Chair: *Peter Verhaert*

- 16:10 **Eric D. Dodds**, University of Nebraska - Lincoln
“Vibrational Activation / Dissociation of Multivalent Cationized Oligosaccharides and their Electron Transfer Products: Prospects for Rapid Regioisomer Differentiation”
- 16:30 **Daniel Figeys**, University of Ottawa
“New MS method for the study of protein glycosylations”
- 16:50 **Ankit Sinha** and Thomas Kislinger, University of Toronto
“Integrating N-glycoproteomics and patient xenografts for identifying novel serum biomarkers for high grade serous ovarian cancers”
CSMS Travel Award – sponsored by SCIEX
- 17:10 **Jon Amster** University of Georgia
“Examining protein-glycosaminoglycan interactions using ion-mobility mass spectrometry”
- 17:30 Discussion
- 18:00 Reception/Dinner
Mount Temple C

Gas Phase Ion Chemistry

Chair: *Paul Mayer*

- 19:30 **Terrance McMahon**, University of Waterloo
“Energetics, Structure and Vibrational Spectra of gaseous Cluster Ions”
Fred Lossing Award Lecture

20:00 **Brandon Santiago** and Gary Glish, The University of North Carolina at Chapel Hill “*Using Tandem Mass Spectrometry to Understand the Fragmentation of Peptides inside a Differential Ion Mobility Spectrometer*”
Marg Northcott Lake Louise Student Travel Award

20:20 **Peter B. Armentrout**, University of Utah
“*What can the BOQ tell us about peptide fragmentation?*”

20:40 **Kristina Håkansson**, University of Michigan
“*Negative Ion Tandem Mass Spectrometry*”

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

Yasaman Jami-Alahmadi and Travis Fridgen, Memorial University of Canada
“*Structure thermochemistry and reactivity studies of metal ion coordinated proline containing peptides in the gas phase*”

Stephen Sciuto and Rebecca Jockusch, University of Toronto
“*Förster Resonance Energy Transfer (FRET) measurements to probe the conformation of gaseous oligonucleotide duplexes in a quadrupole ion trap mass spectrometer*”

Paul M. Mayer, University of Ottawa
“*Dual Electrospray Synthesis and Reactions*”

Michael McDonell, Mandel Scientific
“*Enhancing ion sampling efficiency, ion transmission and detection on a triple quadrupole platform*”

Marcus Kim, Agilent Technologies
“*Screening and Quantitation of 240 Pesticides in Difficult Food Matrices Using the Agilent 6545 Q-TOF Mass Spectrometer*”

Jean-Francois Roy, Agilent Technologies
“*Robust and Sensitive Quantitation of Alprazolam and Midazolam in Plasma using a New Triple Quadrupole Instrument*”

Robert Haufler, SCIEX
“*N geometry TOF analyzer for ESI QqTOF*”

Rosa I. Viner and Arkadi Krainev, Thermo Fisher Scientific
“*Optimization of LC/MS intact /top-down protein analysis on an Orbitrap Fusion mass spectrometer*”

Wendy Cheung, Canadian Food Inspection Agency
“*Finding Pesticides in Popular Beverage Using UHPLC/ESI-MS/MS and QuEChERS*”

Chunyan Hao, Christy Morrissey, Kerry M. Peru, Jonathan Bailey, Jessica Fehr, Allan Cessna and **John V. Headley**, University of Saskatchewan

“Interlaboratory comparison of two methods: ESI/MS/MS analysis of neonicotinoid insecticides in Canadian Prairie Agricultural Wetlands”

Karl Jobst, Ontario Ministry of the Environment and Climate Change

“A quadrupole time-of-flight mass spectrometer coupled to (multidimensional) gas chromatography using atmospheric pressure chemical ionization: analysis of environmental samples by GC/MS using an LC/MS instrument”

Donald J. Douglas, University of British Columbia, Vancouver, BC

Robert K. Boyd, National Research Council of Canada, Halifax, Nova Scotia

“Peter H. Dawson, May 28, 1937-June 12, 2015”

Modupeola A. Sowole and **Lars Konermann**, The University of Western Ontario

“Interactions of Hemoglobin and Myoglobin with their Ligands CN, CO, and O₂ Monitored by Electrospray Mass Spectrometry”

FRIDAY, DECEMBER 4

Nucleic Acids Chair: *Kristina Hakansson*

- 8:00 **Daniele Fabris**, University at Albany, State University of New York
“MS-based epitranscriptomics: new roles for ion mobility and fragmentation techniques”
- 8:25 **Patrick Limbach**, University of Cincinnati
“Mapping RNA Modifications on the Epitranscriptome by LC-MS/MS”
- 8:50 **Valerie Gabelica**, INSERM/University of Bordeaux
“Duplex and quadruplex DNA in the gas phase: novel insights from ion mobility spectrometry and electron photodetachment dissociation MS/MS”
- 9:15 **Mary Rodgers**, Wayne State University
“Tandem Mass Spectrometry Approaches for Probing the Structures and Intrinsic Glycosidic Bond Stability of DNA and RNA Nucleosides”
- 9:40 Discussion and Coffee Break
Victoria Ballroom – Red Room

Proteomics Chair: *Gary Glish*

- 10:10 **Julian Whitelegge**, University of California, Los Angeles
“Improving Coverage of Membrane Proteins in Proteomics”
- 10:30 **Christof Rampitsch**, Agriculture and Agri-Food Canada
“Redox-Sensitive Proteins are Targeted by NADPH Oxidase in *Fusarium graminearum*”
- 10:50 **Frederic Lamoliatte** and Pierre Thibault, Institute for Research in Immunology and Cancer
“Parallel SUMO/Ubi Profiling in Human Cells Using an Optimized Peptide IP”
CSMS Travel Award – sponsored by Thermo Fisher Scientific
- 11:10 **Peter Verhaert**, Delft University of Technology
“TBA”
- 11:30 **Zhongming (Lucas) Hu**, University of Toronto
“Global Survey of Protein Complexes in the Nematode *C. elegans* (WormMap)”
NSERC CREATE Travel Award
- 11:50 Discussion
- 12:00 Lunch
Fairview Dining Room
- Friday Afternoon: Free time – Enjoy the Great Outdoors!
- 18:00 Cocktails
Red Room / Victoria Ballroom
- 19:00 Banquet
Victoria Ballroom

SATURDAY, DECEMBER 5

Toxins, Metabolites, and Environmental Applications

Chair: *Lars Konermann*

- 8:30 **Dajana Vuckovic**, Concordia University, Montreal, QC
"TBA"
- 8:50 **Daniel Beach**, National Research Council
"Differential mobility spectrometry in analysis of algal biotoxins"
- 9:10 **Mark W. Sumarah**, Agriculture and Agri-Food Canada
"Data independent acquisition-digital archive: Moving beyond targeted mycotoxin analysis"
- 9:30 **Brigitte Simons**, SCIEX
"Quantitative Flux Metabolomics for the Investigation of Intracellular Metabolism"
- 9:50 **Kyle Duncan** and Chris Gill, Applied Environmental Research Labs
"Selective positive ion tandem mass spectrometry for rapid screening of carboxylic acids from complex samples using barium ion chemistry and on-line membrane exchange"
CSMS Travel Award – sponsored by Waters
- 10:10 Discussion and Coffee Break
Victoria Ballroom – Red Room

Novel Instrumentation and Methods

Chair: *Peter Verhaert*

- 10:40 **Romain Huguet**, Thermo Fisher Scientific
"Orbitrap Fusion Lumos Tribrid MS, the Most Sensitive Orbitrap MS Ever Made"
- 11:00 **Nidia Lauzon** and Pierre Chaurand, University of Montreal
"High resolution silver assisted LDI imaging MS to monitor the molecular composition of latent fingerprints towards forensic applications"
- 11:20 **Jeffrey Smith**, Carleton University
"Trimethylation enhancement using ¹³C-diazomethane (¹³C-TrEnDi): Increased sensitivity and selectivity of phosphatidylethanolamine phosphatidylcholine"
- 11:40 Matthew T. Campbell, Kenny Chen, Brandon G. Santiago and **Gary Glish**, Department of Chemistry, University of North Carolina
"Differentiating Sugars by Ion/Molecule Reactions and Differential Ion Mobility Spectrometry/Mass Spectrometry"
- 12:00 Discussion and Adjournment
- 12:15 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 vacant.