

LAKE LOUISE XXXI

31st Workshop on Tandem Mass Spectrometry

THURSDAY, NOVEMBER 29

8:00 Introductory Remarks: *Lars Konermann*

Metabolomics 1

Chair: *David Schriemer*

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 *Randy Arnold*, SCIEX
“*Novel Scanning Tools for Simultaneous Quantitative and Qualitative Untargeted Metabolomics Workflow*”

9:45 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*², *K.H. Brian Lam*¹, *Justin Kai-Chi Lau*^{1,2}, *Cheuk-Kuen Lai*¹, *Alan C. Hopkinson*¹
¹Department of Chemistry and Centre for Research in Mass Spectrometry, York University; and
²Department 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**^{1, 2}, **Eric Bonneil**¹, and **Pierre Thibault**², ¹Institute for Research in Immunology and Cancer, University of Montreal, Montreal, QC; ²Department of Chemistry, University of Montreal, Montreal, QC; ³Univ. 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 **Charlie Schmidt**, 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, and R. Subramaniam, S. Chatur, U. Fernando, M. Joshi, L. Wang, Agriculture & Agri-Food Canada, Morden, MB, Canada

“Redox-Sensitive Proteins are Targeted by NADPH Oxidase in Fusarium graminearum”

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”

Lekha Sleno, and Vivaldy Prinville, Université du Québec à Montréal, Montreal QC, Canada

“Quantitative LC-MRM analysis using bile acid kit to study effect of APAP in rat plasma”

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
“Advances in QTOF Technologies Impacting Resolution, Dynamic Range and Mass Accuracy”

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 **Peter Verhaert**, ProteoFormiX, Beerse, Belgium
“Peptidomics: Where Metabolomics and Top-Down Proteomics meet”

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.**