

LAKE LOUISE XXXIII (2021)

33rd International Workshop on Tandem Mass Spectrometry

WEDNESDAY, DEC. 1

5:30 pm to 7:00 pm - Meet & Greet - pick up name tags and drink tickets

Victoria Ballroom Foyer

7:00 pm to 7:30 pm – Networking Reception

Sponsored by:



7:30 pm to 11:00 pm - Dinner

Mount Temple Ballroom A

THURSDAY, DEC. 2

8:00 Introductory Remarks: **Lars Konermann**, The University of Western Ontario, London, ON, Canada

Environmental Applications

Chair: **Gary Glish**, University of North Carolina, Chapel Hill, NC, USA

- 8:05 **Susan Richardson**, Joshua M. Allen, Hannah K. Liberatore, Michael J. Plewa, Elizabeth Wagner, Stuart W. Krasner, Ai Jia, Y. Carrie Guo, and Tiffany Chih-Fen Lee, University of South Carolina, Columbia, SC, USA
What are the drivers of toxicity in U.S. drinking water? Sensitive mass spectrometry methods reveal DBPs of highest concern
- 8:25 Nicholas J. P. Wawryk, Guang Huang, Lindsay K. Jmaiff Blackstock, Junlang Qiu, and **Xing-Fang Li**, University of Alberta, Edmonton, AB, Canada
Mass Spectrometry Identification: What is in your aspartame-sweetened drinks?
- 8:45 **Chris Gill**, Vancouver Island University, Nanaimo, BC, Canada
Advances in Direct Mass Spectrometry for Trace Analysis in Complex Matrices
- 9:05 **Ons Ousji*** and Lekha Sleno, UQAM, Montreal, QC, Canada
Metabolism studies of environmental contaminants by LC-HRMS/MS
***Winner of a Lake Louise Student Travel Award**
- 9:25 **X. Chris Le**, Xiaojian Chen, Tetiana Davydiuk, Karen Hoy, Xiufen Lu, Jordan Schofield, University of Alberta, Edmonton, AB, Canada
Arsenic speciation, exposure, and health effects

9:45 Discussion & Coffee Break

Victoria Ballroom

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Ultrahigh Mass Instrumentation and Methods

Chair: **Jon Amster**, University of Georgia, Athens, GA, USA

- 10:15 **Charlotte Uetrecht**, CSSB Hamburg / University Siegen, Germany
Flying viruses - from biophysical to structural characterization
- 10:40 **Lohra Miller**, Martin Jarrold, Indiana University, Bloomington, IN, USA
Applications of Charge Detection Mass Spectrometry in Molecular Biology
- 11:05 **Joseph Loo**, University of California, Los Angeles, CA, USA
Native Top-Down MS of Large Protein Complexes
- 11:30 Gili Ben-Nissan, Shay Vimer, Jelena Cveticanin, Rivkah Rogawski, Amnon Horovitz and **Michal Sharon**, Weizmann Institute, Rehovot, Israel [via Zoom]
Rapid mass spectrometry investigation of overproduced proteins from crude samples
- 11:55 Discussion
- 12:05 **Workshop group picture**

12:15 to 13:30 Lunch:

Fairview Dining Room

Metabolites

Chair: **Lekha Sleno**, Université du Québec à Montréal, Montreal, QC, Canada

- 14:00 **Erica M. Forsberg**, Myedith Damba, Ellen Kuang, Candice Lambert, San Diego State University, San Diego, CA, USA
Untargeted Metabolomics: Gut Microbial Metabolism of Oral Contraceptives
- 14:20 **Liang Li**, University of Alberta, Edmonton, AB, Canada
High-coverage metabo-lipidome analysis using LC-MS
- 14:40 **Tao Huan**, University of British Columbia, Vancouver, BC, Canada
Recent Improvements of Analytical Accuracy and Precision for Mass Spectrometry-Based Metabolomics
- 15:00 **Alex Birsan**, Waters, Brossard, QC, Canada
Overcoming challenges in analysis of phosphorylated post-translational modification

15:20 Discussion & Coffee Break
Victoria Ballroom

Sponsored by:



Methods and Instrumentation I

Chair: **Peter Verhaert**, ProteoFormiX, Vorselaar, Belgium, The Netherlands

- 15:50 **Margrét Thorsteinsdóttir**, Unnur A. Thorsteinsdóttir, Hrafnhildur L. Runólfssdóttir, Finnur F. Eiríksson, Vidar Ö. Edvardsson, Runólfur Pálsson, Faculty of Pharmaceutical Sciences, University of Iceland, Reykjavik, Iceland
Mass spectrometry-based plasma assay for therapeutic drug monitoring in patients with APRT deficiency

- 16:10 **Yehia Mechref**, Texas Tech University, Lubbock, TX, USA
Derivatization of Sialylated Glycopeptides (DOSG) Enabling Site-Specific Isomeric Profiling using LC-MS/MS
- 16:30 **Steffen Lindert**, Ohio State University, Columbus, OH, USA
Protein Structure Prediction from Mass Spectrometry Data
- 16:50 Brianna Ball, Arianne Bermas, **Jennifer Geddes-McAlister**, University of Guelph, Guelph, ON, Canada
A Systems Biology Approach to Uncovering Mechanisms of Fungal Pathogenesis and Antifungal Resistance
- 17:10 **Rosa Viner**, Thermo Fisher Scientific, San Jose, CA, USA
Improved workflows for structural proteomics on orbitrap platforms
- 17:30 **Daniel Cuthbertson**, Agilent, Seattle, WA, USA
Combatting illegal logging and trafficking of endangered wood species by machine learning statistics using high-resolution LC/MS GC/MS data

18:00 to 19:35 Dinner

Mount Temple Ballroom A

Methods and Instrumentation II

Chair: **Susan Richardson**, University of South Carolina, Columbia, SC, USA

- 19:50 **Lauren Katz***, Michael Woolman, Layla Pires, Mark Zaidi, Stefan O.P. Hofer, Wey Leong, Brad G. Wouters, Danny Ghazarian, An-Wen Chan, Howard J. Ginsberg, Brian C. Wilson, Hal K. Berman and Arash Zarrine-Afsar, University of Toronto, Toronto, ON, Canada,
Picosecond InfraRed Laser-Mass Spectrometry for Rapid Detection of skin Cancers

***CSMS Student Travel Award Winner**

Sponsored by:  Waters
THE SCIENCE OF WHAT'S POSSIBLE.

- 20:10 **Thomas Kislinger**, Princess Margaret Cancer Center, Toronto, ON, Canada
Cell Surface Proteomics for the Detection of Novel Therapeutic Targets

- 20:30 **Randall Purves***, B. O. Shurmer, K. Souster, M. West, C. M. E. Fisher, F. M. Elessawy, Anas El-Aneed, A. Vandenberg, S. Prasad, M. Belford, Canadian Food Inspection Agency, Saskatoon, SK, Canada

Addressing food security challenges with FAIMS Pro

***Fred Lossing Award Winner**

Sponsored by:  Agilent

20:55 Poster Session –authors are asked to be present until 23:00
Victoria Ballroom

Lounes Haroune, Univeristé de Sherbrooke, Sherbrooke, QC, Canada
Toward a Better Understanding of Endogenous Peptide Analysis

Oleg Krokhin, Darien Yeung, Benilde Mizero, Carina Villacrés, Victor Spicer, Rosa Viner, Julian Saba, Bhavinkumar Patel, Sergei Snovida, Penny Jensen, Andreas Huhmer, University of Manitoba, Winnipeg, MN, Canada
Chromatographic properties of peptides labeled with isobaric mass tags in proteomic LC-MS/MS experiments: iTRAQ4, iTRAQ8, TMT, TMTpro

Maggy Lepine, Oriana Zambito and Lekha Sleno, UQAM, Montreal, QC, Canada
Developing a targeted mass spectrometry workflow for investigating the tear proteome

EmmaRae Murphy, David Barnett, Andrew Joy, Susan Budge, Atlantic Cancer Research Institute, Moncton, NB, Canada
An alternative analytical approach for triacylglycerols (TAGs) and their degradation products using LC-FAIMS-MS/MS

Yuen Ki Ng, Elnaz Aliyari, Lars Konermann, The University of Western Ontario, London, ON, Canada,
Protein Aggregation in ESI Droplets and in Bulk Solution

Nastaran Nosrat Tajoddin, Lars Konermann, The University of Western Ontario, London, ON, Canada
Temperature-Dependent HDX-MS Studies of Protein Structure and Dynamics

Rachel Pryce, Hooman Bagheri, Alan C. Peterson and Pierre Chaurand, Université de Montréal, Belleville, ON, Canada,
Relative quantitation of the myelin basic protein in mouse spinal cord tissue sections by MALDI imaging MS

David Schriemer, Andrew Michael, Bruno Amaral, University of Calgary, Calgary, AB, Canada
FIX-MS: In situ crosslinking for interactomics

Pablo Scrosati, Victor Yin, Lars Konermann, The University of Western Ontario, Antigonish, ON, Canada
Hydrogen/Deuterium Exchange Measurements May Provide an Incomplete View of Protein Dynamics: a Case Study on Cytochrome c

Amanda Toupin, Pierre-Luc Mallet and François Corbin, Université de Sherbrooke, Sherbrooke, QC, Canada
LC-MS/MS Development and Validation of a Quantitative Analysis of Potential Peptides Biomarkers Associated to Fragile X Syndrome

Premy Shanthamoorthy, Hannes Röst, University of Toronto, Markham, ON, Canada
High-throughput Lipidomics using Ion-mobility enhanced DDA and DIA Mass Spectrometry

Thomas Walker, David H. Russell, Texas A&M University, College Station, TX, USA,
GroEL: Variable-temperature ESI Native MS studies of GroEL-ATP Binding Thermodynamics and Stabilities

Alexander Haack, W. Scott Hopkins, University of Waterloo, Waterloo, ON, Canada
Predicting Differential Mobility from First Principles

Lekha Sleno, Timon Geib, Makan Golizeh, Ghazaleh Moghaddam, Aimee Supinski, UQAM, Montreal, ON, Canada

Combining untargeted and targeted mass spectrometry to confirm protein modifications in vivo following acetaminophen administration

Peter Verhaert, Kenneth Verheggen, Nivedita Bhattacharya; Remco Crefcoeur; Samruddhi Chawan; Marthe Verhaert; Bram Goossens, ProteoFormiX, Vorselaar, Belgium, The Netherlands

MSHC for single cell peptidomics in Homo sapiens FFPE biobanks

Jeffrey Smith, Carleton University, Ottawa, ON, Canada

Improvements to the LC/MS-based detection of lipids using iTrEnDi

Jeffrey M. Manthorpe, Samiksha Vij, Karl V. Wasslen, Jeffrey C. Smith, Carleton University, Ottawa, ON, Canada

Enhancing the MS-based sensitivity of phosphopeptides via Trimethylation Enhancement using Diazomethane (TrEnDi)

Nour Mashmoushi, Neville Coughlan, Bradley B. Schneider, Yves Le Blanc, Mircea Guna, W. Scott Hopkins, University of Waterloo, Waterloo, ON, Canada

The Spectroscopic Investigation of Differential Mobility Selected Tricyclic Antidepressant Isomers

Darien Yeung, Victor Spicer, Oleg Krokhin, Manitoba Centre for Proteomics and Systems Biology, Winnipeg, MB, Canada

Maximizing MS/MS Cycle Efficiency via boosting Separation Orthogonality in LC/CZE/IMS-MS/MS systems of various configurations

Florence Roux-Dalvai, CHUQ - Université Laval, Quebec City, QC, Canada

Ultrafast bacterial detection in Urine using high-throughput proteomics and artificial intelligence

Jean-Philippe Couture¹, Jean-François Noël¹, Victoria Miller², Sara Little² and Hugo Gagnon¹. 1- PhenoSwitch Bioscience, Sherbrooke, QC, Canada. 2- Proteoform Scientific, Halifax, NS, Canada.

In-depth analysis and optimization of the ProTrap XG sample preparation device using quantitative DIA mass spectrometry.

Ayat Zagzoog, Deborah Michel, Thaisa M. Sandin, Andrew Roebuck, Melissa Herdzyk, Timothy J. Onofrychuk, Dan L. McElroy, Quentin Greba, John Howland, Robert Laprairie, University of Saskatchewan, Saskatoon, SK, Canada

Development and Validation of an LC-MS/MS Method for Quantifying Cannabinoid Levels Following High THC Cannabis Smoke Exposure.

FRIDAY, DEC. 3

Lipidomics

Chair: **Jeff Smith**, Carleton University, Ottawa, ON, Canada

8:00 **Erin S. Baker**, Melanie T. Odenkirk, Kaylie I. Kirkwood, Brian S. Pratt, Nicholas Shulman, Kaipo Tamura, Michael J. MacCoss, Brendan X. McLean, North Carolina State University, NC, USA

Combining Micropunch Histology and Multidimensional Lipidomics Measurements for In-Depth Tissue Mapping

- 8:25 **Ken Stark**, Juan J. Aristizabal-Henao, Klaudia E. Steckel, University of Waterloo, Waterloo, ON, Canada
Using Nutritional Lipidomics to Understand the Impact of Diet on Health
- 8:50 **Steffany Bennett, Irina Alecu**, Miroslava Cuperlovic-Culf, University of Ottawa, Ottawa, ON, Canada
Lipidomic-Based Insights into Disease Mechanisms: A Targeted Lipidomics Discovery Pipeline for Network Analysis
- 9:15 **Gavin Reid**, University of Melbourne, Parkville, Australia [via Zoom]
Advanced Mass Spectrometry Tools for Illuminating the Structural Complexity of the Lipidome
- 9:40 **Matthew Stone**, Mackenzie J. Pearson, Jason Causon, Paul Norris, Christie Hunter, Takashi Baba, SCIEX Manchester-by-the-Sea, MA, USA
Using EIEIO as a novel fragmentation technique for complete lipid characterization in a complex matrix

10:00 Discussion & Coffee Break
Victoria Ballroom

Biological Applications

Chair: **David Schriemer**, University of Calgary, Calgary, Canada

- 10:30 **Dajana Vuckovic**, Lise Cougnaud; Antoine St-Amant; Andreas Bergdahl, Concordia University, Montreal, QC, Canada
Elucidating the role of oxylipins during the diet-induced development of atherosclerosis
- 10:50 Yousef Risha, Vanessa Susevski, Nico Huttmann, Suttinee Poolsup, Zoran Minic, and **Maxim V. Berezovski**, University of Ottawa, Ottawa, ON, Canada
Breast Cancer-Derived Microvesicles Are the Source of Functional Metabolic Enzymes as Potential Targets for Cancer Therapy
- 11:10 **Christopher Thibodeaux**, McGill University, Montreal, QC, Canada
Emergence of Mass Spectrometry for Mechanistic Characterization of Antimicrobial Peptide Biosynthesis
- 11:30 **Antoine Dufour**, Daniel Young, Luiz de Almeida, Laura Edgington-Mitchell, University of Calgary, Calgary, AB, Canada
Playing the game of Pac-Man: Be careful when running with molecular scissors
- 11:50 **Discussion**

12:00 to 13:30 Lunch
Fairview Dining Room

Friday Afternoon: Free time – Enjoy the Great Outdoors!

18:00 Cocktails
Victoria Foyer / Victoria Ballroom

19:00 to 23:00 Banquet
Victoria Ballroom

SATURDAY, DEC. 4

Gas Phase Ions


Chair: **Lars Konermann**, The University of Western Ontario, London, ON, Canada

- 8:00 **Paul M. Mayer**, Bethany Lowe, Juana Salas, Alejandro Cardona, Maxi Burgos-Paci, University of Ottawa, Ottawa, ON, Canada
Exploring the pyrolysis of atmospheric species by mass spectrometry and synchrotron radiation
- 8:20 **Rachel Loo**, Carter Lantz, Benqian Wei, Jessie Li, Wonhyeuk Jung, Joseph Loo, UCLA, Los Angeles, CA, USA
Entropy in Dissociating Complexes
- 8:40 **Christian Ieritano***, J. C. Yves Le Blanc, Bradley B. Schneider, Alexander Haack, Justine R. Bissonnette, W. Scott Hopkins, University of Waterloo, Waterloo, ON, Canada
Protonation-Induced Chirality Drives Separation by Differential Ion Mobility Spectrometry: The Curious Case of Verapamil
***CSMS Student Travel Award Winner** Sponsored by: 
- 9:00 **Francisco Fernandez-Lima**, K. Jeanne Dit Fouque, S. Miller, M. Santos D. Leyva Bombuse, Y. L. Cintron-Diaz, D. Kaplan, V. G. Voinov, M. Ridgeway, Florida International University, Miami, FL, USA
Characterization of middle-down proteoforms using TIMS-UVPD/ECD-TOF MS/MS
- 9:20 **Elnaz Aliyari*** and Lars Konermann, The University of Western Ontario Student, London, ON, Canada
Atomistic Insights into the Formation of Nonspecific Protein Complexes During Electrospray Ionization
***Marg Northcott Lake Louise Student Travel Award Winner**
- 9:40 Discussion & Coffee Break
Victoria Ballroom

Methods and Instrumentation III

Chair: **David Schriemer**, University of Calgary, Calgary, AB, Canada

- 10:10 **Feng Qin**, PerkinElmer, Clayton, CA, USA
LC-MS/MS Applications
- 10:30 Florian Meier, Andreas-David Brunner, Max Frank, Annie Ha, Isabell Bludau, Eugenia Voytik, Stephanie Kaspar-Schoenefeld, Markus Lubeck, Oliver Raether, Nicolai Bache, Ruedi Aebersold, Ben C. Collins, **Hannes L. Röst** & Matthias Mann, University of Toronto, Toronto, ON, Canada
Improved Sensitivity and Duty Cycle of data-independent acquisition (DIA-MS) proteomics using Ion Mobility Separation

- 10:50 **Arjun Sukumaran***, Jennifer Geddes-McAlister, Hannah West, Samanta Pladwig, University of Guelph. Guelph, ON, Canada
Global dual perspective infectome profiling of Klebsiella pneumoniae defines the intricate relationship between host and pathogen
***CSMS Student Travel Award Winner**
- Sponsored by: 
- 11:10 **Jon Amster**, University of Georgia, Athens, GA, USA
Top-down MS for studying protein glycosylation
- 11:30 **Donald Douglas**, University of British Columbia, Vancouver, BC, Canada
The first ICP-MS/MS experiment
- 11:50 **Gary Glish** and Tiffany Crawford, University of North Carolina, Chapel Hill, NC, USA
Differentiating Δ 9-THC from CBD and Δ 8-THC via solvent adduction and MS/MS
- 12:10 Discussion and Adjournment

12:15 to 13:30 Lunch
Fairview Dining Room

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