

# LAKE LOUISE XXXIV

## 34<sup>th</sup> International Workshop on Tandem Mass Spectrometry (2022)

WEDNESDAY, NOV. 30

4:30 pm to 6:30 pm - Meet & Greet - pick up name tags and drink tickets.

*Victoria Ballroom Foyer, First Floor*

6:30 pm to 7:30 pm – Networking Reception

Sponsored by:



7:30 pm to 11:00 pm - Dinner

*Victoria Ballroom*

THURSDAY, DEC. 1

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

### Clinical Mass Spectrometry

Chair: **Peter Verhaert**, ProteoFormiX, Beerse, Belgium

8:05 **Russ Grant**, Labcorp, Burlington, USA

*The Immeasurable Impact of the Triple Quadrupole in Patient Care; Past, Present and Future*

8:30 **Judith Steen**, Boston Children's Hospital, Boston, USA

*Using Tandem MS to decipher Neurodegeneration*

8:55 **Nestor Solis**, AbCellera, Vancouver, BC, Canada

*Keeping pace with a pandemic - Mass spectrometry as part of an integrated antibody discovery and development engine*

9:20 **Amanda Khoo**, Zhuyi Qiu, Vladimir Ignatchenko, Meinusha Govindarajan, Brian Main, Danny Vesprini, Julius O. Nyalwidhe, Stanley Liu, O. John Semmes, Paul C. Boutros, Thomas Kislinger, University of Toronto, Toronto, Canada

*Proteomic landscape of urine-derived extracellular vesicles for risk stratification of localized prostate cancer*

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

9:40 Discussion & Coffee Break

*Victoria Ballroom*

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### Ion Mobility

Chair: **Derek Wilson**, York University, Toronto, ON, Canada

10:10 **Facundo Fernandez**, Georgia Institute of Technology, Atlanta, GA, United States

*Ion Mobility Mass Spectrometry for Unknown Metabolite Identification: Hope or Hype?*

- 10:30 **Alexander Haack**, University of Waterloo, Waterloo, ON, Canada  
*First Principles Modelling of Ion-Solvent Clustering in Ion Mobility* sponsored by   
**Winner of a CSMS Travel Award**
- 10:50 **Karl Jobst**, Mahin Hashemihedeshi, Amber McNeil, Xiaolei Li,  
 Meera Bissram, Jake Breen, Frank Dorman, Memorial University of Newfoundland, St. John's, NFLD, Canada sponsored by   
*Gas chromatography x cyclic ion mobility mass spectrometry: a novel platform that enables the discovery of emerging contaminants*
- 11:10 **Jonathan Krieger**, Tharan Srikumar, Robin Park, Christopher Adams, Sven Brehmer  
 Bruker Canada, Milton, ON, Canada  
*PaSER: A Complete Real-Time CCS Enabled Bioinformatics Solution for timsTOF data*
- 11:30 **John Sausen**, Jim Prell, University of Oregon, Brandon Ruotolo University of Michigan, Blaine Roberts; Emory University, Sheher Mohsin; Agilent Technologies, Kaylie Kirkwood, University of North Carolina, Erin Baker; University of North Carolina, John Fjeldsted; Agilent Technologies  
*Recent Advances in Ion Mobility? Solving unsolved problems.*
- 11:50 Discussion  
 Workshop group picture

12:00 to 13:30 Lunch

*Fairview Dining Room*

**Biological Applications**

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

- 13:40 **Lei Tian**, Caren Akiki, Lan Liu, Shaghig Bilamjian, Tarun Anumol, Daniel Cuthbertson, Stéphane Bayen, McGill University, Ste-Anne-de-Bellevue, QC, Canada  
*Identification of honey fingerprints for the botanical classification using a non-targeted LC-QTOF-MS method*  
**Winner of a CSMS Travel Award** sponsored by 
- 14:00 **Antoine Dufour**, Nabanghu Das, Luiz de Almeida, University of Calgary, Calgary, AB, Canada  
*Tryptase b regulation of joint lubrication and inflammation via proteoglycan-4 in osteoarthritis*
- 14:20 **Lohra Miller**, Martin Jarrold, Benjamin Draper, Indiana University, Bloomington, IN, USA  
*Deciphering the Charge Profile of Megadalton Sized dsDNA Plasmids with Charge Detection Mass Spectrometry*
- 14:40 **Lekha Sleno**, Ons Ousji, Ikram Benhadji Serradj, UQAM, Montreal, QC, Canada  
*Exposomics analysis in urine: custom spectral library to detect metabolites of environmental contaminants*
- 15:00 **John McLean**, Vanderbilt University, Nashville, TN, USA

*Advanced phenomics with structural mass spectrometry*

15:20 **Sylvain Letarte**, Phytronix Instruments Inc., Calgary, AB, Canada  
*How to invite Samhsa to your Christmas party without ruining it*

15:40 Discussion & Coffee Break  
**Victoria Ballroom**

**Proteomics and Metabolomics**

Chair: **Peter Verhaert**, ProteoFormiX, Beerse, Belgium

16:10 **Nicholas Prudhomme**, Jennifer Geddes-McAlister, David Overy, Mike D. McLean, Doug Cossar, University of Guelph, Guelph, ON, Canada  
*Bacterial growth-mediated proteome remodeling of *Nicotiana benthamiana* defines unique signatures modulating target production in molecular pharming*

16:30 **Maggy Lépine**, Oriana Zambito, Jean-Yves Sahyoun, Marie-Claude Robert and Lekha Sleno, University of Quebec at Montreal, Montreal, QC, Canada  
*An innovative targeted workflow for measuring quantitative changes in the tear proteome of patients with common and rare eye diseases*  
**Winner of a Lake Louise Travel Award**

16:50 **Nathan Yates**, University of Pittsburgh, Pittsburgh, PA, United States  
*Implementation, Optimization, and Pre-Validation of High-performance Plasma Amyloid- $\beta$  Biomarkers for Alzheimer's Disease*

17:10 **Rene Zahedi**, Beckmann L, Berg V, Dickhut C, Hallek M, Frenzel L, Zahedi RP, University of Manitoba, Winnipeg, MB, Canada  
*Protein mass spectrometry identifies MARCKS as marker for the differential response to Bruton tyrosine kinase (BTK) inhibitors in chronic lymphocytic leukemia (CLL) patients*

17:30 **Robert DiLorenzo**, SCIEX, Concord, ON, Canada  
*A multi-acquisition-mode strategy for in-depth metabolomics analysis*

17:50 Discussion

18:00 to 19:15 Dinner  
**Mount Temple Ballroom A**

**Metabolites and Toxins**

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

19:30 **Justin Renaud**, Agriculture and Agri-Food Canada, London, ON, Canada  
*Diagnostic Fragmentation Filtering: Linking natural product discovery with ion fragmentation*  
**Winner of the CSMS Young Investigator Award**

sponsored by



19:50 **Dajana Vuckovic**, Elissa Mariani, Irina Slobodchikova, Concordia University, Montreal, QC, Canada

*Mapping human metabolism of mycotoxins using LC-MS/MS*

20:10 **J. Rafael Montenegro-Burke**, University of Toronto, Toronto, ON, Canada  
*Mapping of the Human Cell Metabolome Reveals Novel Targets for Cancer Therapies*

20:30 **Liang Li**, University of Alberta, Edmonton, AB, Canada  
*Tandem MS for deep metabolome characterization*

21:10 **Poster Session** –authors are asked to be present until 23:00

**Benjamin Muselius**, Jennifer Geddes-McAlister, Florence Rou-Dalvia, Arnaud Droit, University of Guelph, Guelph, ON, Canada  
*Quantitative Proteomic Profiling of Splenic Response to Fungal Infection*

**Marcus Kim**, Mark Sartain, Valery G. Voinov, Joseph Meeuwsen, Christian Klein and Joseph S. Beckman, Agilent Technologies, Mississauga, ON, Canada  
*Fine structural elucidation of phospholipids with practical electron-based fragmentation on QTOF instruments*

**Peter Tieleman**, Beibei Wang, University of Calgary, Calgary, AB, Canada  
*Release of lipid nanodiscs from charged nano-droplets in the electrospray ionization process*

**Christof Rampitsch**, Slavica Djuric-Ciganovic, Mei Huang, Zhen Yao, Mark Lubberts, Agriculture & Agri-Food Canada - Morden Research Station, Morden, MB, Canada, Peter Verhaert  
Proteomix, Beerse, Belgium,  
*Identifying endogenous rust peptides using top-down peptidomics, de novo sequencing and bioinformatics strategies*

**Joe Binkley**, David Alonso, LECO, St. Joseph,  
*Comprehensive Screening of Pollutants in Household Dust Using High-Resolution Mass Spectrometry with Enhanced Chromatographic Resolution*

**Oleg Krokhine**, Darien Yeung, Vic Spicer, University of Manitoba, Winnipeg, MB, Canada  
*2D HPLC / CZE applications in bottom-up proteomics: peptide separation orthogonality for 20+ different 2D combinations*

**Ons Ousji**, Mbarka Bchetnia, Catherine Laprise, Lekha Sleno, UQAM, Montreal, QC, Canada  
*Integrating metabolomics, proteomics and transcriptomics data to decipher molecular perturbation in Epidermolysis bullosa simplex, a rare skin disease*

**Achille Cappiello**, M. Dutt, A. Arigo, P. Palma, G. Famiglioni, University of Urbino, Urbino, Italy

*Development of an LC-MS/MS method using a liquid electron ionization interface in negative chemical ionization mode for the analysis of per- and polyfluoroalkyl substances*

**Pablo Scrosati**, Lars Konermann, The University of Western Ontario, London, ON, Canada  
*Mechanism of Peptide Retention in Reversed-Phase Liquid Chromatography with Water/Acetonitrile Gradient Elution*

**John Headley**, Jessica Fehr, Christy Morrissey, Dena McMartin, University of Saskatchewan, Saskatoon, SK,  
*Tandem MS of neonicotinoids in bird plasma*

**David Schriemer**, University of Calgary, Calgary, AB, Canada  
*Advanced methods for in situ crosslinking*

**Lydia Liu**, Chenghao Zhu\*, Paul C. Boutros, Thomas Kislinger, University of Toronto, Toronto, ON, Canada  
*Expanding the Prostate Cancer Proteome: Custom Databases for Noncanonical Peptides*

**Jennifer Geddes-McAlister**, Reid Buchanan, Michael Woods, Kerry Woolnough, Arianne Bermas, University of Guelph, Guelph, ON, Canada  
*Proteomics of Fungal Disease in One Health*

**Lise Cougnaud**, Antoine St-Amant, Andreas Bergdahl, Dajana Vuckovic, Concordia University, Montreal, QC, Canada  
*Analysis of the atherogenicity of low carbohydrate - high protein diets using longitudinal oxylipin profiling in murine plasma*

**Hafiza Jawaria Munir**, Torsten Kleffmann, Sally P.A. McCormick, University of Otago, Dunedin, New Zealand,  
*Proteomic analysis to study the effect of 4-phenylbutyrate treatment on ABCA1 function and trafficking*

**Bernard Delanghe**, Thermo Fisher Scientific, Bremen, Germany  
*Boosting the identification and quantification rates by AI driven data acquisition and processing strategies.*

**Christian Ieritano**, Alexander Haack, W. Scott Hopkins, University of Waterloo, Bolton, ON, Canada  
*Kinetic vs Thermodynamic Control within Differential Mobility Spectrometry - An Unexpected Observation from Alpha Acids found in Brewing Hops*

**Joshua Roberts**, Elena Godbout, Christopher Boddy, Jean-Simon Diallo, Jeffrey C. Smith, Carleton University, Ottawa, ON, Canada  
*Elucidating the lipidomic dynamics of lentiviral infection*

**Jeff Smith**, Christian Rosales, Krysten Sheedy, Samuel Shields, Natalie Whitmore, Karl Wasslen, Jeffrey Manthorpe, Carleton University, Ottawa, ON, Canada  
*Addressing the glyphosate paradox using iTrEnDi*

**Derek Wilson**, Cristina Lento; Esther Wolf, York University, Toronto, ON, Canada  
*On the evolution of distinct specificity profiles in protein families with highly similar structures*

**Peter Verhaert**, Dick Swaab, Marc Ramael, Kenneth Verheggen, Nivedita Bhattacharya, Marthe Verhaert, Raf Sciot, ProteoFormiX, Beerse, Belgium  
*Multi-omics imaging of human FFPE tissue sections with single cell resolution: complementing the human biomolecular tissue atlas.*

**Jessica Fehr**, Sonia Cabezas, John V. Headley, Christy Morrissey, Chunyan Hao, Ian Vander Meulen, Kerry M. Peru, Environment Climate Change Canada, Saskatoon, SK, Canada  
*Neonicotinoids and other Pesticides from Bird Plasma by LC MS/MS*

**Adamo Young**, Bo Wang, Hannes Röst,  
*MassFormer: Tandem Mass Spectrum Prediction using Graph Transformers*

**Christian Bleiholder**, Florida State University, Florida, USA  
*Structure-elucidation by ion mobility / mass spectrometry: experimental & theoretical approaches*

**Lars Konermann**, University of Western Ontario, London, ON, Canada  
*Mechanism of Magic Number Cluster Formation During Electrospray Ionization*

## FRIDAY, DEC. 2

### Legends of Lake Louise

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

- 8:00 **Graham Cooks**, Purdue University, West Lafayette, IN, USA  
*Accelerated Reactions in Microdroplets: Mass Spectrometry for Synthesis and Analysis*
- 8:25 **Catherine Costello**, Boston University School of Medicine, Boston, MA, USA  
*The Past is Prologue; The Future is Now!*
- 8:50 **Mike Bowers**, UCSB, Santa Barbara, CA, USA  
*Assembly of Amyloid Peptides*
- 9:15 **Alan Marshall**, Florida State University, Tallahassee, FL, USA  
*Current Techniques and Applications of Fourier Transform Ion Cyclotron Resonance MS/MS*
- 9:40 Discussion & Coffee Break  
**Victoria Ballroom**

### Gas Phase Ion Chemistry

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

- 10:10 **Kristina Hakansson**, Eunju Jang, Steven DeFiglia, Menatallah Youssef, University of Michigan, Ann Arbor, MI, USA  
*Mobile Proton Control for Enabling Sulfoproteomics*
- 10:30 **Victor Ryzhov**, K.Parker, A. Fanizza, Northern Illinois University, Dekalb, IL, USA  
*Sustainable hydrocarbon production from fatty acids studied by gas-phase ion chemistry*
- 10:50 **Francisco Fernández-Lima**, Florida International University, Miami, FLA, USA  
*Development of top double down tandem IMS - UVPD/ECD - MS strategies for proteoform characterization*
- 11:10 **Ian Webb**, Melanie Cheung, See Kit, Indiana University-Purdue University, Indianapolis, MI, USA  
*New Directions in Tandem Mass Spectrometry Applied to Protein Structure*
- 11:30 **Jon Amster**, University of Georgia, Athens, GA, USA  
*Ion Mobility Study of The Roundabout Protein and Its Heparan Sulfate Complex*

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. 3**

**Environmental Applications**

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

8:00 **Susan Richardson**, Alexandria Forster, Ying Zhang, Danielle Westerman , University of South Carolina, Columbia, SC, US

*Capturing the PFAS Footprint: LC-MS/MS vs. a New Total Organic Fluorine Method*

8:20 **Sébastien Sauvé**, Université de Montreal, Montreal, QC, Canada

*Per- and polyfluoroalkyl substances (PFAS) in the environment*

8:40 **X. Chris Le**, Alekasandra Popowich, Xiaowen Yan, Xiufen Lu, Qingqing Liu, Hanyong Peng, Xing-Fang Li, University of Alberta, Edmonton, AB, Canada

*A mass spectrometry study of arsenic binding to p53*

9:00 **Susana Kimura Hara**, Md Fahim Hossain, Jorge Pérez Pérez, University of Calgary, Calgary, AB, Canada

*Benzotriazoles: chlorination and their role in the formation of disinfection byproducts*

9:20 **Xing-Fang Li**, Caley Craven, Kristin Carroll, Nicholas Wawryk, University of Alberta, Edmonton, AB, Canada

*Smelling Tap Water and Amino Acids during Spring Runoffs*

9:40 Discussion & Coffee Break


*Victoria Ballroom*

**Methods and Instrumentation**

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

10:10 **Philip Britz-McKibbin**, Ritchie Ly, McMaster University, Hamilton, ON, Canada  
*Untargeted Serum Lipid Profiling by Multisegment Injection-Nonaqueous Capillary Electrophoresis-Mass Spectrometry: Identifying Biomarkers of Omega-3 Index*



- 10:30 **Shipei Xing**, Sam Shen, Banghua Xu, Tao Huan, The University of British Columbia, Vancouver, BC, Canada  
*Bottom-up MS/MS interrogation enables large-scale discovery of unreported molecular formulae with significance control*  
**Winner of a CSMS Travel Award,** sponsored by 
- 10:50 **Adriana Arigo**, Nicole Marittimo, Genny Grasselli, Giorgio Famiglini, Pierangela Palma, Mansoor Saeed, Simon Perry, Pablo Navarro, Phil Clarke, Mark Brittin, Achille Cappiello, University of Urbino, Urbino, Italy  
*Exploring the advantages of coupling liquid electron ionization LC-MS interface with high-resolution mass spectrometry: a powerful strategy for component identification in complex matrices*
- 11:10 **Chris Gill**, Vancouver Island University, Nanaimo, BC, Canada  
*High Throughput Paper Spray Mass Spectrometry for Clinically Relevant Diagnostics*
- 11:30 **Chad Weisbrod**, Karl W. Smith, Lissa C. Anderson, Carla Harkin, Diego F. Cobice, Christopher L. Hendrickson, National High Magnetic Field Laboratory, Tallahassee, FLA, United States  
*Cost-free Tandem MS Coupled with 21 T FT-ICR Mass Spectrometry Imaging*
- 11:50 **Gary Glish**, University of North Carolina, Chapel Hill, NC, USA  
*DiffN - A new approach to MS/MS data dependent acquisition*
- 12:10 Discussion and Adjournment

12:15 to 13:30 Lunch

**Fairview Dining Room**

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