

LAKE LOUISE XXXIV

34th 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**, Zhuyu 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

Sponsored by:



Your local gas generation partner

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 Steno**, 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- β 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

20:30 **J. Rafael Montenegro-Burke**, University of Toronto, Toronto, ON, Canada
Mapping of the Human Cell Metabolome Reveals Novel Targets for Cancer Therapies

20:50 **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
Proteoformix, 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. Famiglini, 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

We gratefully acknowledge financial support for the Lake Louise Workshop
(Sponsorship levels are ranked in accordance with the Lake Louise downhill ski runs)

“Black Diamond” Sponsor



Agilent



ThermoFisher
SCIENTIFIC

Waters

THE SCIENCE OF WHAT'S POSSIBLE.

“Blue” Sponsors



MOBILion
SYSTEMS, INC.



Phytronix

“Green” Sponsors



CREATIVE MOLECULES INC.

EVUSEP



Parker **BALSTON**
Analytical Gas System Products
(formerly Whatman Analytical Gas Systems Products)

PEAK
SCIENTIFIC
Your local gas generation partner



Western 