# Lake Louise Tandem MS Workshop Preliminary Program



December 3 - 6, 2025

Fairmont Chateau Lake Louise 111 Lake Louise Drive Lake Louise, AB, Canada

## **Welcome to the Lake Louise Tandem MS Workshop**

Dear Colleagues,

Welcome to the 37th edition of the Tandem MS Workshop. We hope that you will enjoy the presentations and the social events we have organized for you this year. Held annually at the Fairmont Chateau Lake Louise, Lake Louise, Alberta, the Workshop focuses on scientific exchange and dissemination of technical aspects of tandem mass spectrometry.







37th Annual Tandem Mass Spectrometry Workshop

#### **General Information**

#### Registration

Registration Opens on Wednesday, December 3 at 16:00 in the Victoria Ballroom Foyer. Please come to pick up your packages and badges.

#### **Posters**

Poster presenters should have their posters up by 20:00, Wednesday, December 3. Posters must be taken down by noon on Friday, December 5.

#### Meals

Please note: If you order beverages other than tea or coffee at <u>ANY</u> meal, you will be charged. If anyone has special dietary requirements, please contact Janette Champ, if you have not already done so. Vouchers are available for lunches on Friday and Saturday for those wishing to ski or hike. Please obtain the Lunchto-Go Vouchers <u>at dinner the night before.</u> Vouchers are to be used at the Chateau Deli located in the Lobby of the Hotel. If you take a voucher, you may NOT join in the sit-down lunch as well.

## Wednesday, December 3

16:00 to 18:30 Meet & Greet

17:00

Pick up program package, name tags, drink tickets.

Victoria Ballroom Foyer
Networking Reception

Victoria Ballroom Foyer

18:00 to 20:00 Buffet Dinner

Victoria Ballroom

19:00 Introductory Remarks: *David Schriemer*, The University of Calgary, Calgary, AB, Canada

Victoria Ballroom

19:05 to 19:50 *Plenary Lecture - Victoria Ballroom* 

Neil Kelleher, Northwestern University, Evanston, IL, USA

TBA

## Thursday, December 4

07:00	Breakfast Louiza, Lower Level
07:30	Registration Opens for Late Badge Pickup Victoria Ballroom Foyer
	<u>Metabolomics</u> Chair: <b>Erin Baker</b> , University of North Carolina, Chapel Hill, NC, USA
08:00	Emma Schymanski, LCSB, University of Luxembourg, LUX Open Science Approaches for Mass Spectrometry-Based Exposomics
08:25	Vincent Charron-Lamoureux, Marta Sala-Climent, Abubaker Patan, Shipei Xing, Ipsita Mohanty, Yasin El Albiead, Maribeth R. Nicholson, Mindy Engevik, Thomas Horvath, Monica Guma, Andrew Patterson, Pieter C. Dorrestein, University of California-San Diego, CA, USA Reverse metabolomics enables public data mining and reveals a drug/bile acid conjugate in inflammatory diseases
08:50	Roger Linington, Simon Fraser University, Vancouver, BC, CAN The Impact of Mass Analyzer Advancements on Natural Products Metabolomics WATERS Sponsored Talk

09:15 *Liang Li*, University of Alberta, Edmonton, AB, CAN

Recent advances in tandem mass spectrometry for deep metabolomics

09:40 <u>Discussion & Coffee Break</u>

Victoria Ballroom

# Thursday, December 4, cont.

	<u>Spatial MS</u> Chair: <b>Peter Verhaert</b> , Leuven University, Leuven, BEL
10:10	Livia Schiavinato Eberlin, Baylor College of Medicine, Huston, TX, USA Medical Mass Spectrometry to Advance Patient Care
10:35	<i>Nicolai Slavov</i> , Northeastern University and Parallel Squared Technology Institute, Cambridge, MA, USA, <i>Increasing proteomics throughput by multiplexing in the mass and time domains</i>
11:00	Bernhard Spengler, Carolin Morawietz, David Luh, Karl Christian Schaefer, Stefanie Gerbig, Max A. Mueller, Alina Schindler, Carmen Paschke, Kerstin Strupat, Justus Liebig University, Giessen, DEU New data acquisition and analysis approaches in high-resolution MS2 and MS3 imaging of biological samples
11:25	Pierre Chaurand, Samarth Gangoo, Université de Montréal, Montreal, QC, CAN Mass spectrometry imaging of the gut microbiome INGENIO Sponsored Talk
11:50	Benjamin Muselius, Bruno Amaral, Christina Pan, Spencer Funk, Pauline Douglas, David Schriemer, University of Calgary, Calgary, AB, CAN Development of a Spatial Proteomics Platform with Sub-cellular Resolution. Winner of a CSMS Travel Award, Sponsored by Thermo Fisher Scientific
12:10	Discussion & Group Photo  Meet at top of stairs for Group Photo
12:30 - 14:00	Lunch Louiza, Lower Level
	<u>Computational MS</u> Chair: <i>Lars Konermann</i> , University of Western Ontario, London, ON, CAN
14:00	Cailum Stienstra, Emir Nazdraji, Tao Huan, W. Scott Hopkins, University of Waterloo, Waterloo, ON, CAN From RP to HILIC: Graph Transformers Power Method-Independent Prediction of Retention Times for Metabolomics Annotation Winner of the Bill Davidson Award, Sponsored by the Davidson Family
14:20	Hannes Rost, Adamo Young, Fei Wang, David S Wishart, Bo Wang, Russell Greiner, Hannes Rost, University of Toronto, Toronto, ON, CAN FraGNNet: A Deep Probabilistic Model for Tandem Mass Spectrum Prediction
14:40	David Weil, Agilent, Santa Clara, CA, USA Best Practices in Nontargeted Data Analysis Workflows and Compound Identification AGILENT Sponsored Talk

Thursday, December 4, cont.		
15:00	Steffen Lindert, University of California, Los Angeles, CA, USA In silico assessment of potential protein structural distortion by covalent labeling reagents	
15:20	Mathieu Lavallée-Adam, Maram El-Azouni, Giorgio Freije, Jonathan Krieger, Tharan Srikumar, University of Ottawa, Ottawa, ON, CAN A Novel Machine Learning Approach for Real-Time Assessment of Precursor Ion Identifiability in Mass Spectrometry-Based Proteomics	
15:40	Discussion & Coffee Break Victoria Ballroom	
	Environmental Chair: Jeff Smith, Carleton University, Ottawa, ON, CAN	
16:10	<b>Sébastien Sauvé</b> , Université de Montréal, Montreal, QC, CAN <i>PFAS are everywhere in our water, food, soils, sewage sludge and air? what's next?</i>	
16:30	Erin Baker, Kara Joseph, Ashlee Falls, James Dodds, Michael Powers, University of North Carolina at Chapel Hill, Chapell Hill, NC, USA Is There a Correct Way to Milk a Dolphin? Examining Maternal Contaminant Transfer	
16:50	Matthew D. Stone, SCIEX, Concord, ON, CAN New Technology to Transform Your Translational Research: Introducing the ZenoTOF 8600 System SCIEX Sponsored Talk	
17:10	Elliot Wright, Daniel G. Beach, Pearse McCarron, National Research Council of Canada Increasing Confidence and Comparability in LC-HRMS Non-Target Analysis of Marine Algal Toxins	
17:30	Discussion	
18:00 to 19:15	Dinner Mount Temple AB	
	PICK UP LUNCH-TO-GO VOUCHERS. Please ask a server	
	Proteomics Chair: Dave Schriemer, University of Calgary, Calgary, AB, CAN	
19:30	Daniel Figeys, Leyuan Li, Kai Cheng, Janice Mayne, Zhibin Ning, Xu Zhang, Alain Stintzi, Quadram Institute, Norwich, GBR Drug-microbiome interactions by metaproteomics Winner of the CSMS Fred Lossing Award, Sponsored by Agilent	

Qiaomu Li, Xin Liu, Mohana Talasila, R. Glen Uhrig, University of Alberta, Edmonton,

Using Integrated Proteomics Analysis to Characterize Roles of Splicing Kinasel (SK1) in

Winner of a CSMS Travel Award, Sponsored by Waters

19:55

AB, CAN

Arabidopsis thaliana

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## Thursday, December 4, cont.

20:15 *Nestor Solis*, Thermo Fisher Scientific

TBA

#### **THERMO Sponsored Talk**

20:35 *Leonard Foster*, University of British Columbia, Vancouver, BC, CAN

Simultaneous single-cell proteomics and lipidomics to understand astrocyte biology

#### Thursday, Dec. 4 Poster Session

20:55 to 23:00 Authors are asked to be present until 23:00

Lucas Abruzzi, Jack Gillies, Erik T. Krogh, Daniel G. Beach, Chris G. Gill, Centre for Health and Environmental Mass Spectrometry (CHEMS), Vancouver Island University, Nanaimo, Quantitative Multiclass Cyanotoxin Screening by Paper Spray Mass Spectrometry

*Radwa Asar*<sup>1</sup>, Maria Alejandra Oviedo-Ludena<sup>2</sup>, KarinaChimbo Huatatoca<sup>2</sup>, LipuWang<sup>2</sup>, Randy Kutcher<sup>2</sup> and Anas Elaneed<sup>1</sup>.

<sup>1</sup>College of Pharmacy and Nutrition, University of Saskatchewan, Saskatoon, SK, CAN

<sup>2</sup>Department of Plant Sciences, University of Saskatchewan, Saskatoon, SK, CAN Improving Canadian Cereal Grains, Detecting and Quantifying Toxic Deoxynivalenol Derivatives

Joseph Corstvet, David Lewis, Carter Asef, Dmitry Leontyev, Xin Ma, Rebecca Arnold, John A. Petros, Facundo M. Fernández, Georgia Institute of Technology, Atlanta, GA, USA Triboelectric Nanogenerator-Powered Laser Ablation/Nanoelectrospray Ionization (TENG LAESI) Mass Spectrometry Ion Source

Mahsa Dolatkhah Ouch Bolagh, Lars Konermann, University of Western Ontario, London, ON, CAN Modelling Electrospray Operation in a Charged Emitter Using Molecular Dynamics Simulations

Broc Glover, Waters Corporation, Mississauga, ON, CAN Leveraging High Speed MRT Analyzers for Faster MS Imaging Without Sacrificing Sensitivity

Kasra Hanifi, Lars Konermann, University of Western Ontario, London, ON, CAN Protein Release from Ammonium Acetate-Containing Droplets during Native Electrospray Ionization: Insights from Mobile-Proton Molecular Dynamics Simulations

John Headley, Erin Pederson, Rio Bouwers, Ian J. Vander Meulen, Dena W. McMartin, Cassidy VanderSchee, Environment and Climate Change Canada, Saskatoon, SK, CAN Orbitrap mass spectrometry of oil sands metal naphthenates

Angelina Jaeger, Haley Tomlin, Joseph Monaghan, Chris G. Gill, Erik T. Krogh, Centre for Health and Environmental Mass Spectrometry, Nanaimo, BC. CAN Driven by Data: Mobile Tandem Mass Spectrometry for In-field Monitoring of Tire-Derived Aquatic Toxicant

*Haley Jostes*, University of North Carolina – Chapel Hill, Chapel Hill, NC, USA Understanding the Lipidome of Human Plasma Extracellular Vesicles / Emerging Particles of Interest for Clinical Applications

#### Thursday, Dec. 4 Poster Session, cont.

Amir Khajavinia, Amir Khajavinia, Deborah Michel, Jordan Reekie, Udoka C. Ezeaka, Randy W. Purves, Robert B. Laprairie, Anas El-Aneed, University of Saskatchewan, Saskatoon, SK, CAN Analysis of Psilocin Using Quantitative LC-MS/MS and Qualitative Nanodiamond-based MALDI-MS

*Thomas Kislinger*, Princess Margaret Cancer Center, Toronto, ON, CAN *Pan-cancer N-glycoproteomic atlas of patient-derived xenografts for surface protein discovery* 

Chris Le, Tetiana Davydiuk, Juanjuan Fu, Xiufen Lu, Jagdeesh Uppal, University of Alberta, Edmonton, AB, CAN

Biomarker of susceptibility for arsenic-induced health effects

Xing-Fang Li, Di Zhang, Qiming Shen, Tingting Zhao, Khac Ngoc Minh, Tongtong Xiang, University of Alberta, Edmonton, AB, CAN

Nontargeted analysis of water contaminants

**Evelyn Mackay-Barr**, Lars Konermann, University of Western Ontario, London, ON, CAN Probing the Effects of Covalent Oxidative Modifications on Protein Stability and Dynamics

Jocelyn Menard, Joshua A. Roberts, Jacob Clarke, Karlye Rudd, Jeffrey C. Smith, Carleton University, Ottawa, ON, CAN

Liquid Chromatography Mass Spectrometry Fatty Acid Data Extraction (LC-MS FADE): Leveraging Untargeted Lipidomics Data for Fatty Acid Profiling

Joseph Monaghan, Tian Zhao, Kiera Nguyen, Madison Schiyuk, Helena Petrosova, Dave Goodlett, Julian Lum, Kyle Duncan, Vancouver Island University, Nanaimo, BC, CAN

Multimodal Imaging of Methionine Cycle Metabolites and Immune Cell Markers in Ovarian Tumors by nanospray-Desorption Electrospray Ionization (nano-DESI)

Feng Qin, Holly Lee, Phenomenex, Torrance, CA, USA Practical Strategies for Analysis Short Chain PFAS with LC-MS/MS

*Tanya Sharma*, *Kumari Anshu*, *Tuong Van Nguyen*, *Sonal K. Thengane*, *Hilkka Kenttamaa*, Purdue University, West Lafayette, IN, USA

Reaction Mechanisms for Fast Pyrolysis of Polystyrene by Using a Pyroprobe Integrated With an Ion Trap Mass Spectrometer

Samuel Shields, Kathrine Daniel, Izabella A Pena, Children's Hospital of Eastern Ontario, Ottawa, ON, CAN Targeted LC-MS Profiling of Vitamin B6 Metabolism in SLC19A1 Knockout K562 Cells

**Peter Verhaert**, Gilles Frache, Marco Giampà Raf Sciot, Bart Ghesquière, Leuven University, Leuven, BEL AP/MALDI and DESI high-resolution MS histochemistry for FFPE biobank tissue analysis aligned with pathology practice

*Emily Vincent*, *James N. Dodds; Haley C. Jostes; Allison N. Fry; Erin S. Baker*, University of North Carolina - Chapel Hill, Durham, NC, USA

Mood-Altering Waters: A Multidimensional Investigation of Antidepressant Contamination in Surface Water

# Friday, December 5

07:00	Breakfast Louiza, Lower Level
	Fundamentals and Ion Chemistry Chair: Gary Glish, University of North Carolina, Chapel Hill, NC, USA
08:00	Peter Armentrout, Samantha K. Walker, Tobias Dijkhuis, Marissa Keeler, Brandon C. Stevenson, Giel Berden, Jonathan Martens, Jos Oomens, University of Utah, Salt Lake City, UT, USA
	Influence of Methylating the Serine Side-chain on the Decomposition of Protonated Asparaginyl Serinen using GIBMS, IRMPD, and Theoretical Modeling
08:20	Robert Rider, Carter Lantz, David H. Russell, Texas A & M University, College Station, TX, USA
	Hydration-Dependent Conformational Landscape of CI-2 Measured with vT-IM-MS Winner of the Margaret Northcott Lake Louise Travel Award
08:40	Victor Ryzhov, Northern Illinois University, DeKalb, IL, USA Structure and reactivity of radical ions
09:00	Kirsty Yuen Ki Ng <sup>1</sup> , Quinn W. Currie <sup>2</sup> , Elnaz Aliyari <sup>1</sup> , Caroline Cui <sup>1</sup> , Siavash Vahidi <sup>2</sup> and Lark Konermann <sup>1</sup> The University of Western Ontario, London, ON, Canada <sup>2</sup> University of Guelph Guelph, ON, Canada Can Enzymes Retain Catalytic Activity in the Gas Phase? Insights from ESI-IMS/MS/MS and Mobile-Proton Molecular Dynamics Simulations  Legends of Lake Louise Travel Award Winner
09:20	Kristina Hakansson, Menatallah M. Youssef, Neven N. Mikawy, Kuan-Lu Wu, Lissa C. Anderson NHMFL/Florida State University, Tallahassee, FL, USA Improved Annotation of Atypical Fragment Ions: From Sulfotyrosine to Antibodies
09:40	<u>Discussion &amp; Coffee Break</u> Victoria Ballroom
	Methods and Instrumentation Chair: Kicki Hakansson, NHMFL/Florida State University, Tallahassee, FL, USA
10:10	Francisco Fernandez-Lima, Florida International University, Miami, FL, USA Characterization of linker and core histones using TIMS-UVPD-FT-ICR MS/MS
10:30	Houssain El Aribi, Zef Scientific Inc., Laval, QC, CAN Practical Use of LC-MS/MS for Routine Screening, Confirmation and Quantitation: The Good, The Bad, and The Ugly ZEF SCIENTIFIC Sponsored Talk
10:50	Chris Gill, Taelor M. Zarkovic, Lucas R. Abruzzi, Jindar N.S. Sboto, Jack Gilles, Jason L. Robinson, Daniel G. Beach, Centre for Health and Environmental Mass Spectrometry - Vancouver Island University, Nanaimo, BC, CAN Recent Advances in Clinical, Environmental and Forensic Paper Spray Mass Spectrometry

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### Friday, December 5, cont.

11:10 Lydia Zamlynny, Elliott J. Wright, Rob C. Jamieson, Daniel G. Beach, Dalhousie University,

Wolfville, NS, CAN

Non-Target Tandem Mass Spectrometry Methods for Analysis of Cyanobacterial Secondary

Metabolites

Winner of a CSMS Travel Award, Sponsored by SCIEX

11:30 *Yehia Mechref*, Texas Tech University, Lubbock, TX, USA

Automated and Accurate Glycan and Glycopeptide Quantitation by Parallel Reaction Monitoring

Based LC-MS/MS

11:50 <u>Discussion</u>

12:00 to 13:30 Lunch

Louiza, Lower Level

FRIDAY AFTERNOON - FREE TIME - ENJOY THE GREAT OUTDOORS!

18:00 <u>Cocktails</u>

Victoria Foyer/Victoria Ballroom

19:00 to 23:00 Banquet Dinner

Victoria Ballroom

PICK UP LUNCH-TO-GO-VOUCHERS. Please ask a server.

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# Saturday, December 7

07:00	Breakfast Louiza, Lower Level
	Biomarkers and Disease Chair: Xing-Fang Li, University of Alberta, Edmonton, AB, CAN
08:00	Christoph Borchers, McGill University / Lady Davis Institute, Montreal, QC, CAN SysQuan: democratize absolute quantitative analysis of the human proteome
08:20	Margret Thorsteinsdottir, Kristrun Y. Holm, Kari Arnarsson, Valdis Gunnarsdottir Thormar, Sigridur K. Bodvarsdottir, Yassene Mohammed, Christoph H. Borchers and Finnur F. Eirkiksson, Faculty of Pharmaceutical Sciences, University of Iceland, Reykjavik, ISL High-throughput tandem mass spectrometry assay for absolute quantification of protein biomarkers of human diseases
08:40	<b>Lekha Sleno</b> , Nathan Ghafari, Sherin Nawaito, Danielle Berber, Charlotte Usselman, Nicolas Pilon, UQAM, Montreal, QC, CAN High coverage metabolomics applied to investigating perturbations related to polycystic ovary syndrome
09:00	TBA
09:20	TBA
09:40	<u>Discussion &amp; Coffee Break</u> Victoria Ballroom
	<u>Methods and Instrumentation – 2</u> Chair: <b>Jeff Smith</b> , Carleton University, Ottawa, ON, CAN
10:10	Jon Amster, Jonathan Choi, University of Georgia, Athens, GA, USA Glycosaminoglycan Analysis by Capillary Zone Electrophoresis and Tandem MS
10:30	Richard Oleschuk, Jess Deng, Jennifer Klowich, Jian Yu, Kyla Toshack, Mina Alidoust, Rachel Wood, Malek Hassan, Avena Ross, Queen's University, Kingston, ON, CAN An ambient ionization approach to monitor spatiotemporal dynamics of microbial metabolites
10:50	Kyle Duncan, Nicholas Woytowich, CatherineRoberts, Phillip Ankley, Markus Brinkmann, Erik Krogh, Vancouver Island University, Nanaimo, BC, CAN Uncovering Spatially Resolved 6PPDQ Metabolism in Rainbow Trout Fry with Nano-DESI Mass Spectrometry Imaging

## Saturday, December 7, cont.

11:10 Ziqin Ni, Konstantin Ayzikov, Alexander Makarov, Kyle Fort, Facundo M. Fernandez, Georgia

Institute of Technology, Atlanta, GA, USA

LC-Orbitrap Collision Cross Section Measurements to Improve Annotation in Non-Targeted

Lipidomics

11:30 TBA

11:50 Gary Glish, Cameron D. Worthington, Tyler S. Larson, University of North Carolina, Chapel Hill,

NC, USA

Is What Comes Out of Your ESI Source What You See in Your Mass Spectrum?

12:10 <u>Discussion and Adjournment</u>

12:15 to 13:30 Lunch

Louiza, Lower Level

FOR INDIVIDUAL STAYING ON:

SATURDAY AFTERNOON - FREE TIME - ENJOY THE GREAT OUTDOORS!

18:00 <u>Dinner</u>

Victoria Foyer/Victoria Ballroom

## **Sunday, December 8**

07:00 to 10:30 Breakfast

Louiza, Lower Level

Thank you for joining us at the 37th Annual Lake Louise Tandem MS Workshop. We hope you will join us next year!

## **Our Sponsors**

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





















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