Lake Louise Tandem MS Workshop

Program

November 29 to December 2, 2023

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 35th 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, the workshop focuses on scientific exchange and dissemination of technical aspects of tandem mass spectrometry.



35th Annual Tandem Mass Spectrometry Workshop

General Information

Registration
Registration Opens on Wednesday, November 29 at 16:00 in the Victoria Ballroom Foyer. Please come to pickup your packages and badges.

Posters
Poster presenters should have their posters up by 20:00, Wednesday, November 29. Posters must be taken down by noon on Friday, December 1.

Meals
Please note: If you order beverages other than tea or coffee at **ANY** 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 Lunch-to-Go Vouchers **at dinner the night before.** 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, November 29

16:00 to 19:00 **Meet & Greet**
Pickup program package, name tags, drink tickets
Victoria Ballroom Foyer

18:00 to 19:30 **Networking Reception**
Victoria Ballroom Foyer

19:30 to 23:00 **Dinner**
Victoria Ballroom

20:25 Introductory Remarks: ***Lars Konermann,*** The University of Western Ontario, London, ON, Canada

20:30 to 21:15 ***Plenary Lecture - Victoria Ballroom***
John Yates, The Scripps Research Institute, La Jolla, CA
How a single mutation in CFTR causes the systemic disease Cystic Fibrosis: Interactions, PTMs, Structure

Thursday, November 30

07:00 **Breakfast**
Louiza, Lower Level

07:30 Registration Opens for Late Badge Pickup
Victoria Ballroom Foyer

08:00 to 9:40 ***Fourier Transforms and Tandem Mass Spectrometry***
Chair: *Jonathan Amster*, University of Georgia, Georgia, USA

08:00 ***Kathrin Breuker***, University of Innsbruck, Innsbruck, Austria
Native top-down MS of RNA-ligand complexes for binding site mapping

08:25 ***Ljiljana Paša-Tolić***, Pacific Northwest National Laboratory, Richmond, Washington, USA
Advancing spatial and cellular omics with FTMS

08:50 ***Peter O'Connor,*** University of Warwick, UK
Two-Dimensional Mass Spectrometry

09:15 ***Evan Williams***, University of California, Berkeley, California, USA
Rapid Protein Melting and Aggregation Measured with Laser Heating Mass Spectrometry

09:40 **Discussion & Coffee Break**
Victoria Ballroom

Thursday, November 30, cont.

10:10 to 12:10 ***Proteins, Part I***
Chair: ***Erin Baker, The University of North Carolina at Chapel Hill***

10:10 ***Siavash Vahidi,*** *Bradley T.V. Davis, Algirdaz Velyvis,* University of Guelph, Guelph, Canada
Fluorinated ethyl amines as electdrospray-compatible neutral pH buffers for native mass spectrometry.
Sponsored by: Waters™

10:30 ***Ian Webb,*** *Rebecca Cain, Melanie Cheung See Kit, Tyler Cropley, Frank Sobott, Christopher Chouinard, Christian Bleiholder*, Indiana University, Indianapolis, United States
Mass Spectrometric Characterization of Chemically and Natively Unfolded Proteins

10:50 ***Steffen Lindert,*** *Ohio State University,* Columbus, USA
Computational Protein Structure Prediction from Mass Spectrometry Data

11:10 ***Madison Turner****, Samuel E. Hoff; Adwaith B. Uday; Algirdas Velyvis; Natalie Zeytuni; Massimiliano Bonomi; Siavash Vahidi,* University of Guelph, Ontario Canada;
Mapping Allosteric Pathways in the M. tuberculosis 20S Proteasome Core Particle using HDX-MS
Sponsored by: Waters™
Winner of a CSMS Travel Award.

11:30 ***Michael Bowers,*** *Xikun Liu, Yingying Jin, Steven Burattto*, UCSB, California, USA
Mechanisms of Assembly, Crosstalk and Therapeutic Agents in Amyloid Diseases

11:50 ***Francisco Fernandez Lima,*** *Florida International University,* Miami, United States
Top Down strategies using complementary HDX, TIMS, and ECD/UVPD MS/MS

12:10 **Discussion & Group Photo**

12:30 to 14:00 **Lunch**
Fairview Dining Room

14:00 to 15:40 ***MS/MS "Omics" Applications***
Chair: ***Peter Verhaert,*** **ProteoFormiX BV**

14:00 ***Brett Larsen,*** ThermoFisher
Orbitrap Astral - Rethink what is possible

14:20 ***Lekha Sleno,*** *UQAM,* Montreal, Canada
Combining targeted and untargeted workflows and correlation analysis for metabolomics studies

14:40 ***Margret Thorsteinsdottir,*** *University of Iceland,* Reykjavik, Iceland
Discovery of novel biomarkers for early breast cancer diagnosis using targeted proteomics

15:00 ***Cate Simmermaker,*** *Karen E. Yannell, Genevieve C. Van de Bittner, and Philip L. Lorenzi,* Agilent Technologies, Santa Clara, United States
End to End Multiomics Analysis for Biological Insights

15:20 ***Tao Huan,*** University of British Columbia, Vancouver, Canada
Addressing big data challenges in MS-based metabolomics

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

Thursday, November 30, cont.

16:10 to 17:30 ***Nonpolar Molecules: Lipids and Metabolites***
Chair: *Jeff Smith,* Carleton University

16:10 ***Victor Ryzhov***, *K. Parker, R. King, R. A. J. O'Hair, A. Canty,* Northern Illinois University, DeKalb, United States
Studying C-H and C-C activation of cyclohexane catalyzed by transition metal complexes in the gas phase

16:30 ***Jian Yu***, *Manasa Ramachandra, Haidy Metwally, Jennifer Kolwich, Hailey A. Tomm, Martin Kaufmann, Rachel Klotz, Chang Liu, J. C. Yves LeBlanc, Thomas R. Covey, Avena C. Ross, Richard D. Oleschuk*, Queen's University, Kingston, Ontario, Canada
From rapid spatial profiling to precise structural elucidation: Mass spectrometry based microbial metabolome analysis
Winner of a CSMS Travel Award Sponsored by: SCIEX

16:50 ***Tingting Yan***, *Zhongling Liang, Boone Prentice,* University of Florida, Florida, USA
Characterization of Phosphatidylcholine Structures Using Collisional Induced Dissociation/ Electron Induced Dissociation (CID/EID)
Winner of the Marg Northcott Lake Louise Travel Award

17:10 ***Alexandria Van Grouw****, Markace A. Rainey, Molly E. Ogle, Johnna Temenoff, Samuel G. Moore, Facundo M. Fernandez,* Georgia Institute of Technology, Atlanta, Georgia, USA
A Machine Learning Approach for Semi-Quantitative Non-targeted Lipidomics
Winner of a Lake Louise Travel Award

17:30 **Discussion**

18:00 to 19:15 **Dinner**
Fairview Dinning Room

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

19:30 to 20:55 ***Proteomics***
Chair: *Derek Wilson, York University*

19:30 ***Christoph Borchers***, McGill University / Lady Davis Institute, Montreal, QC
Using multiple structural proteomics approaches to characterize drug binding sites in proteins
Winner of the CSMS Fred Lossing Award Sponsored by: Agilent

19:55 ***Jennifer Van Eyk,*** Cedars-Sinai Medical Cetner, Los Angeles, USA
Can single cell proteomics help with precision health?

20:15 ***Olivier Julien,*** University of Alberta, Edmonton, Canada
Characterizing post-translational modifications during viral infections

20:35 ***Antoine Dufour,*** *Julian Wolf, Young Joo Sun, Jennifer T Vu, Elena Wang, Alexander G Bassuk MD, Vinit B Mahajan,* University of Calgary, Calgary, Canada
Liquid biopsy proteomics combined with artificial intelligence identifies the cellular drivers of eye aging and disease in vivo

20:55 **Discussion**

Thursday, November 30 Poster Session

21:00 to 23:00 Authors are asked to be present until 23:00

Michael Andersen, *Nicolai Bache, Dorte Bekker-Jensen, Magnus Huusfeldt,* Evosep, Odense C, Denmark
End-to-end automated, LC-MS sample separation workflows improves throughput and reproducibility

Sedigheh Barzegar, *Randy Purves, Anas El-Aneed, C*ollege of Pharmacy and Nutrition, University of Saskatchewan, Saskatoon, Canada
Modernizing LC-MS methods for detection of veterinary drug residues.

Vimanda Chow, *Cristina Lento, Derek J Wilson,* York University, Mississauga, Canada
Using membrane mimics (nanodiscs) to understand the structural and conformational dynamics of membrane proteins by TRESI-HDX-MS

Emma Finch*, Michel, D., Adamko, D., El-Aneed, A.,* University of Saskatchewan , Saskatoon, Canada
Comparison of Normalization Approaches in Targeted Urine Metabolomics, The Use of 'Total' Metabolome vs Creatinine

Christian Ieritano, *Patrick Thomas, W. Scott Hopkins,* University of Waterloo, Bolton, Canada
Argentination: A Silver Bullet for Cannabinoid Separation by Differential Mobility Spectrometry

Oleg Krokhin, *Darien Yeung, Quinn Neale, Ying Lao, Vic Spicer,* University of Manitoba, Winnipeg, Canada
Reversed-phase HPLC behaviour of post-translationally modified peptides in bottom-up proteomic experiments

Jocky Kung, *Tomislav Damjanović, Thomas Kierspel, Charlotte Uetrecht,* Centre for Structural Systems Biology, Hamburg, Germany
Mass Spectrometry as Sample Delivery Platform for Single-Particle Imaging with X-rays and Related Experiments

Maggy Lépine, *Marie-Claude Robert and Lekha Sleno,* University of Quebec in Montreal, Montreal, Canada
Potential diagnostic biomarkers of Sjögren's syndrome from targeted tear proteomics

X. Chris Le, *Tetiana Davydiuk, Karen Hoy, Chester Lau, Qingqing Liu, Xiufen Lu, Hanyong Peng, Michael Weinfeld, Xiaowen Yan,* University of Alberta, Edmonton, Canada
Mass spectrometry enabling environmental health studies of arsenic

Tsun Hei Arthur E. Lee*, Josh Featherstone, Jonathan K. Martens, Terrance B. McMahon, W. Scott Hopkins,* University of Waterloo, Waterloo, Canada
Novel Unimolecular Dissociation of Fluorinated Propionic Acids

Cristina Lento, *Joseph Anacleto, Ayesha Maqsood, Derek J. Wilson,* York University, Toronto, Canada
An Improved Apparatus with On-Line Chromatography for Hydrogen Deuterium Exchange Mass Spectrometry Measurements from Milliseconds to Hours

Xing-Fang Li, *Qiming Shen, Di Zhang, and Nicholas Wawryk,* University of Alberta, Edmonton , Canada
Nontargeted analysis of organic amines in water

Paul Mayer, *Bethany Lowe, Andras Bodi,* University Of Ottawa, Ottawa, Canada
What a Difference a Chlorine Makes: The Remarkably Different Unimolecular Ion Chemistry of Phenyl Formate and Chloroformate

Thursday, November 30 Poster Session, cont.

Benjamin Muselius, *Dr. Jennifer Geddes-McAlister, Dr. Arnaud Droit, Florence Roux-Dalvai,* University of Guelph, Guelph, Canada
Harnessing tandem mass spectrometry-based proteomics to construct a C. neoformans organ atlas

Oluwaseun Ogunniyi, *Radwa Mahmoud, Amir Khajavinia, Deborah Michel, Changiz Taghibiglou and Anas El-Aneed,* University of Saskatchewan, Saskatoon, Canada
Development of Novel LC-MS Method to Detect INDIP, a Novel Peptide for Acne Treatment.

Boone Prentice, University of Florida, Gainesville, USA
High chemical resolution imaging mass spectrometry using gas-phase ion/ion reactions

Christof Rampitsch, *Slavica Djuric-Ciganovic, AAFC; Mei Huang, AAFC; Zhen Yao, AAFC; Mark Lubberts, AAFC (Summerland); Peter Verhaert, Proteoformix, Beerse, Belgium,* Molecular Genetics, Morden, Canada
N-terminal peptidome enrichment and top-down peptidomics identifies potentially novel endogenous rust peptides

Chris Ryan, *Nazdrajic E., Hopkins W. S.,* University of Waterloo, Waterloo, Canada
Novel Separation Method of PFAS via 2-Dimensional LCxDMS

David Schriemer, *Frantisek Filandr, Vladimir Sarpe,* University of Calgary, Chestermere, Canada
Full automation of HX-MS data analysis

Pablo Scrosati, *Lars Konermann,* The University of Western Ontario, London, Canada
Peptide Retention Time Prediction in Reversed-Phase Liquid Chromatography by Molecular Dynamics Simulations

Cailum Stienstra, *Chris Ryan, Justine Bissonette, W. Scott Hopkins,* University of Waterloo, Waterloo, Canada
Improved Prediction of Dispersion Curves using Recurrent Neural Networks (RNNs)

Peter Verhaert, *Maureen Feucherolles, Gilles Frache,* ProteoFormiX BV, Vorselaar, Belgium
Pushing the limits of atmospheric pressure MALDI MS histochemistry on high-resolution Orbitrap mass spectrometers for FFPE biobanked tissue analysis

Benjamin Warnes, *Jasmine Chihabi, Jeffrey Manthorpe,* Carleton University, Ottawa, Canada
Unveiling the Power of Negative Ion Mode ESI-MS: Identifying Species with Remarkable Signal Intensity and Collisional Stability

Oriana Zambito, *Nejia Lassoued, Rodolphe Soret, Nicolas Pilon, Lekha Sleno,* UQAM, Montreal, Canada
Studying the metabolome and proteome of colon and fecal samples using untargeted LC-MS/MS

Chad Weisbrod*, Jesse D. Canterbury, John P. Quinn, Lissa C. Anderson, Amy M. McKenna, Greg T. Blakney, Dan McIntosh, Michael W. Senko, Christopher L. Hendrickson,* NHMFL, Tallahassee, United States
A novel quaternary hybrid Q-Orbitrap-IT-FT-ICR mass spectrometry platform

Christian Rosales, *Krysten L. Sheedy, Karl V. Wasslen, Jeffrey M. Manthorpe, Jeffrey C. Smith,* Carleton University, Ottawa, Canada
Trimethylation enhancement using diazomethane (TrEnDi) enables enhanced LCMS detection of glufosinate and 3-(methylphosphinico)propionic acid from complex canola samples

Joshua Roberts*, Natalie Prowse, Shawn Hayley, Jeffrey, C. Smith,* Carleton University, Ottawa, Canada
Development of a Fatty Acid Methyl Ester Profiling and Total Cholesterol Determination Workflow by GCMS for Mouse Prefrontal Cortex Brain Tissue

Thursday, November 30 Poster Session, cont.

***Sharon Curtis**, Zoran Minic, Tony Durst, Petr Kasyanchyk et al.,* University of Ottawa, Ottawa, Canada
Fatty Acid Content, of the seeds of probably the rarest tree on the planet! PLEODENDRON COSTARICENSE (CANELLACEAE)

***Jeffrey Smith**, Joshua Roberts, Angela Radnoff, Aleksandra Bushueva, Meaghan Harley, Karl Wasslen,* Carleton University, Ottawa, Canada
Understanding factors that contribute to the DARK MATTER of lipidomics datasets

***Derek Wilson**, Cristina Lento; Esther Wolf; Alex Listigovers; Vimanda Chow; Joseph Anacleto,* York University, Toronto, Canada
Mass Spectrometry-enabled Dynamic Structural Biology for Therapeutics Development and Manufacturing

John Headley, *Samuel T. Mutto, Benedict Gannon, Ian Vandermuelen, Dani Degenhardt, Dena W. McMartin, Callan Littlejohn, Hugh E. Jones, Diana Palacio Lozano, Meng Li, Mark P. Barrow,* Environment and Climate Change Canada, Saskatoon, Canada
TimsTOFMS characterization of oil sands naphthenic acid fraction compounds in wetland mesocosms

***Daniel DeBord,** Jordan Stewart, Michelle English, Ashli Simone, Maria Fawaz, Komal Kedia,* MOBILion Systems, Chadds Ford, United States
High Throughput, Label-Free Cyclic Peptide Soft Spot Identification via High Resolution Mobility Aligned Fragmentation Analysis

***Susan Richardson,** Jiafu Li, Md. Tareq Aziz, and Caroline Granger,* University of South Carolina, Colombia, United States
High resolution-MS uncovers new halocyclopentadiene disinfection by-products in drinking water

***Lars Konermann**, Zeyuan Liu, Yousef Haidar, Mathew J. Willians, and Nicholas A. Bainbridge*, The University of Western Ontario, London, Canada
On the Chemistry of Aqueous Ammonium Acetate Droplets during Native Electrospray Ionization Mass Spectrometry

Friday, December 1

07:00 **Breakfast**
Louiza, Lower Level

08:00 to 09:40 ***Ion Activation***
Chair: ***Gary Glish, University of North Carolina***

08:00 ***Glen Jackson,*** West Virginia University, Morgantown, United States
Recent Advances in Charge Transfer Dissociation Mass Spectrometry (CTD-MS)

08:25 ***Kristina Hakansson,*** *Steven DeFiglia, Neven Mikawy, Menatallah Youssef,* University of Michigan, Ann Arbor, United States
Physical and Chemical Approaches to Improved Tandem Mass Spectrometry of Posttranlational Modifications

08:50 ***James Prell,*** *Samantha O. Shepherd, Austin W. Green, Ruwan T. Kurulugama, Kenneth R. Newton,* University of Oregon, Eugene, USA
Ion Heat Transfer, Activation, and Kinetic Energy Damping in Native Mass Spectrometry: Lessons from an Improved Impulsive Collision Model

09:15 ***Scott McLuckey,*** Purdue University, West Lafayette, United States
Dipolar DC Collisional Activation and Ion/ion Reactions for the Structural Characterization of Bio-ions: From Lipids to G-4 Quadruplexes

09:40 **Discussion & Coffee Break**
Victoria Ballroom

10:10 to 11:50 **Methods and Instrumentation, Part I**
Chair: Jeffrey Smith, Carleton University

10:10 ***Jeff Manthorpe****, Benjamin B. Warnes, Jasmine Chihabi,* Carleton University, Ottawa, Canada
Challenging the Dogma: Is Negative Polarity Inherently Less Sensitive Than Positive Polarity?

10:30 ***Patrick Pribil****,* SCIEX, Concord, Canada
Increasing biological insight using alternative fragmentation and high sensitivity MS/MS on the SCIEX ZenoTOF7600 system

10:50 ***Jonathan Amster,*** *Eli Roberts,* University of Georgia, Athens, United States
Mass spectrometric strategies for assigning heavy isotope enrichment in glycoproteins

11:10 ***Nicholas Wawryk,*** *Caley Craven, Kristin Carroll, and Xing-Fang Li,* University of Alberta, Edmonton, Canada
Changes in Natural Organic Matter during Spring Runoff: Implications Disinfection Byproduct Formation
Winner of a CSMS Travel Award Sponsored by: Thermo SCIENTIFIC

11:30 ***Joseph Monaghan****, Angelina Jaeger, Misha Zvekic, Joshua Jai, Haley Tomlin, Jamieson Atkinson, Tanya Brown, Chris Gill, Erik Krogh,* Vancouver Island University, Nanaimo, Canada
Automated high throughput analysis of tire-derived phenylene diamine quinones (PPDQs) in water by online membrane sampling coupled to ESI-MS/MS
Winner of the ETP - Bill Davidson Travel Award Sponsored by: The Davidson Family

11:50 **Discussion**

Friday, December 1, cont.

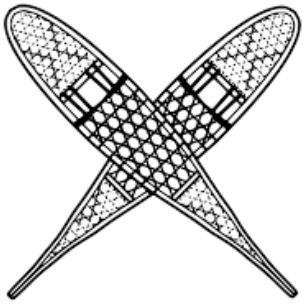
12:00 to 13:30 **Lunch**
Fairview Dining Room

FRIDAY AFTERNOON - FREE TIME - ENJOY THE GREAT OUTDOORS!

18:00 **Cocktails**
Victoria Foyer/Victoria Ballroom

19:00 to 23:00 **Banquet Dinner**
Victoria Ballroom

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



Saturday, December 2

07:00 **Breakfast**
Louiza, Lower Level

08:00 to 9:40 ***Metabolomics, Drugs & Environmental Applications***
Chair: ***Lars Konermann, University of Western Ontario***

08:00 ***Erin Baker,*** *Anna Boatman, James Dodds, Kaylie Kirkwood Donelson, Kylie Rock, Scott Belcher,* University of North Carolina, Chapel Hill, United States
Alligators as Sentinel Species for Environmental and Health Concerns

08:20 ***Sylvain LeTarte,*** Phytronix Instruments Inc.
Reaching the sub-second analysis in mass spectrometry: opening a window to the future

08:40 ***Christopher Chouinard***, Clemson University, Clemson, United States
Ion Mobility-Aligned MS/MS Fragmentation for Identification of Novel Psychoactive Substances

09:00 ***Rafa Montenegro Burke,*** University of Toronto, Toronto, Canada
Untargeted metabolomics illuminates cellular heterogeneity in cancer

09:20 ***Mark Sumarah,*** *Justin Renaud, Natasha DesRochers, Lyne Sabourin,* Agriculture and Agri-Food Canada, London, Canada
Targeted and Non-targeted sampling and LC-MS analysis of surface water for environmental contaminants

09:40 **Discussion & Coffee Break**
Victoria Ballroom

10:10 to 12:10 **Methods and Instrumentation, Part II**
Chair: ***David Schriemer, University of Calgary***

10:10 ***Pierre Chaurand,*** *Rachel Pryce, Hooman Bagheri, Alan C. Peterson ,* Université de Montréal, Montreal, Canada
Spinal cord remodeling across six mouse mutant strains monitored by mass spectrometry imaging

10:30 ***Anas El-Aneed,*** College of Pharmacy and Nutrition, University of Saskatchewan, Saskatoon, Canada
MS-based quantification in pharmaceutical analysis without conventional chromatographic separations, opportunities and limitations

10:50 ***Facundo Fernandez,*** *Daniel Vallejo, Carter Asef, Joseph Cortsvet,* School of Chemistry and Biochemistry. Georgia Institute of Technology, Atlanta, United States
Fundamentals and Applications of Triboelectric Nanogenerator Nanoelectrospray Ionization

11:10 ***Richard Oleschuk,*** *Malek Hassan, Haidy Metwally, Mark McKeown, Matthias Hermann, Rachel Theriault, Jian Yu, Martin Kaufmann, Kevin Y. M. Ren, Randy E. Ellis,* Queen's University, Kingston, Canada
An Ambient Ionization Probe (LMJ-SSP) and Conductive Touch Platform to Profile Fresh, Fresh Frozen and Formalin Fixed Paraffin Embedded Tumour Samples

Saturday, December 2, cont.

11:30	***Chris Gill,*** *Lucas R. Abruzzi; Daniel G. Beach; Erik T. Krogh;* Vancouver Island University, Nanaimo, Canada *Multi-Class, High Throughput Algal Toxin Measurements using Paper Spray Mass Spectrometry*
11:50	***Gary Glish,*** *Cameron D. Worthington,* University of North Carolina, Chapel Hill, USA *IMS/IMS/MS/MS: Is more MS better*?
12:10	**Discussion and Adjournment**
12:15 to 13:30	**Lunch** ***Fairview Dining Room***
12:30 to 15:00	Meeting of the Organizing Committee
	SATURDAY AFTERNOON - FREE TIME - ENJOY THE GREAT OUTDOORS!
18:00	**DINNER**
	Cocktails & Dinner ***Victoria Foyer/Victoria Ballroom***

Sunday, December 3

07:00 to 10:30	**Breakfast** ***Louiza, Lower Level***

Thank you for joining us at the 35th 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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