



19<sup>th</sup> Annual Conference of the Metabolomics Society

# METABOLOMICS

NIAGARA FALLS, CANADA

JUNE 18-22

# 2023

## SCHEDULE OF ORAL PRESENTATIONS



# AGENDA AT A GLANCE

Metabolomics in Health and Disease

Technology Advancements

Mental Health, Drug Addiction and Medicinal Cannabis

Computational Metabolomics, Statistics & Bioinformatics

Plants, Food, Environment and Microbes

SUNDAY, JUNE 18			
	Peller A	Peller C	Peller D
11:00 a.m.	REGISTRATION OPEN		
12:00 p.m. – 2:00 p.m.		W1: Ion Mobility Mass Spectrometry Workflows for Metabolomics	W2: Future Potential of Metabolomics for Illuminating the Molecular Dark Matter of Soil
2:00 p.m. – 2:15 p.m.	BREAK		
2:15 p.m. – 4:15 p.m.	W3: Meta-analysis, biomarker discovery, and pathway analysis of metabolomics data	W4: Emergent Technologies in NMR Metabolomics	
4:30 p.m. – 6:30 p.m.	W5: Hands-on analysis of ms-based met and exposomics big data using ADAP	W6: Multi-Platform Metabolomics Workflows	W7: EMN – Professional Career Development
6:45 p.m. – 7:45 p.m.	Career Night – Job Fair   The Lounge		
7:45 p.m. – 9:00 p.m.	Career Night – Roundtable Discussions   Peller B		
MONDAY, JUNE 19			
	Peller A	Peller C	Peller D
7:30 a.m.	REGISTRATION / INFO DESK OPEN		
8:15 a.m. – 10:15 a.m.	W8 Part 1: MetaboAnalyst 5.0 for high-throughput LC-MS	W9: Moving Toward Consensus: mQACC Community on Best QA/QC Practices	W10: Data preprocessing in non-targeted metabolomics
10:15 a.m. – 10:30 a.m.	BREAK		
10:30 a.m. – 12:30 p.m.	W8 Part 2: MetaboAnalyst 5.0 for high-throughput LC-MS	W11: Interdisciplinary Metabolomic Epidemiology: Pathway to Clinical Translation	W12: Data Standardization and Reuse through Public Repositories
12:30 p.m. – 1:45 p.m.	LUNCH BREAK – ON YOUR OWN		
1:45 p.m. – 3:15 p.m.	Opening Ceremony & Plenary Session 1 – Lorraine Brennan   Fallsview		
3:15 p.m. – 3:30 p.m.	BREAK		
	Fallsview	Peller C	Peller D
3:30 p.m. – 5:15 p.m.	1 Diet and Nutrition	2 In-Depth and Real-Time Analysis	3 Metabolite Annotation and Identification
5:15 p.m. – 6:45 p.m.	Welcome Reception – Poster Session 1		
7:00 p.m. – 8:00 p.m.	Metabolomics Society Town Hall Meeting   Fallsview		
8:00 p.m. – 9:00 p.m.	MANA Networking Reception   The Lounge		
TUESDAY, JUNE 20			
	Fallsview	Peller C	Peller D
7:45 a.m.	REGISTRATION / INFO DESK OPEN		
8:30 a.m. – 9:30 a.m.	Plenary Session 2 – Marja Lamoree   Fallsview		
9:30 a.m. – 10:15 a.m.	BREAK		
10:15 a.m. – 12:00 p.m.	4 Cardiovascular and Metabolic Diseases	5 Novel Methods in Metabolomics	6 Non-targeted Analysis in Biomonitoring
12:00 p.m. – 1:30 p.m.	LUNCH BREAK AND SPONSOR PRESENTATIONS		
12:20 p.m. – 1:20 p.m.	Sponsor Pres: SCIEX	Sponsor Pres: Agilent Technologies	Sponsor Pres: Metabolon
1:30 p.m. – 3:15 p.m.	7 Cancer	8 Multi-omics and Meta-analysis	9 Foodomics and Food Security
3:15 p.m. – 3:30 p.m.	BREAK		
3:30 p.m. – 5:15 p.m.	10 Vendor Session	11 Neurological Disorders and Medicinal Cannabis	12 Microbial Metabolomics
5:15 p.m. – 6:45 p.m.	Poster Session 2		
6:45 p.m. – 7:45 p.m.	WomiX + FeMS Mixer   The Lounge		
7:00 p.m. – 8:30 p.m.	EMN Reception   Peller AB		
WEDNESDAY, JUNE 21			
	Fallsview	Peller C	Peller D
8:00 a.m.	REGISTRATION / INFO DESK OPEN		
8:30 a.m. – 9:30 a.m.	Plenary Session 3 – Gary Patti   Fallsview		
9:30 a.m. – 10:15 a.m.	BREAK		
10:15 a.m. – 12:00 p.m.	13 Microbiome	14 Reproducibility and QA/QC	15 Ecosystem Metabolomics and Exposomics
12:00 p.m. – 1:30 p.m.	LUNCH BREAK – ON YOUR OWN		
12:20 p.m. – 1:20 p.m.	Sponsor Pres: Thermo Fisher Scientific	Sponsor Pres: Bruker Scientific	
1:30 p.m. – 3:15 p.m.	16 Epidemiology	17 New Advances in Lipidomics	18 Plant Metabolomics I
3:15 p.m. – 3:30 p.m.	BREAK		
3:30 p.m. – 5:15 p.m.	19 Lung and Respiratory Diseases	20 High-throughput and Spatial Metabolomics	21 Data Processing and Machine Learning
5:15 p.m. – 6:45 p.m.	Poster Session 3		
7:30 p.m. – 11:00 p.m.	Conference Dinner		
THURSDAY, JUNE 22			
	Fallsview	Peller C	Peller D
8:15 a.m.	REGISTRATION / INFO DESK OPEN		
8:30 a.m. – 9:30 a.m.	Plenary Session 4 – Susan Murch   Fallsview		
9:30 a.m. – 10:30 a.m.	Poster Session 4		
10:30 a.m. – 12:15 p.m.	22 Pregnancy, Maternal and Neonatal Health	23 Plant Metabolomics II	24 Data Harmon. and Metabolic Networks
12:30 p.m. – 2:00 p.m.	Plenary Session 5 – Caroline Johnson – Awards and Closing   Fallsview		
2:00 p.m.	BOX LUNCH TO GO		

## ★ AWARD WINNERS

Monday, June 19		
Time	Session	Abstract #
1:45 p.m. – 3:15 p.m.	<b>Opening Ceremony and Plenary Session 1</b> Metabolomics for Nutrition Research <i>Lorraine Brennan, University College Dublin, Ireland</i>	<i>Fallsview</i>
3:30 p.m. – 5:15 p.m.	<b>Session 1. Diet and Nutrition</b> <i>Session Chairs: Susan Sumner and Susana Palma</i>	<i>Fallsview</i>
3:30 p.m. – 4:00 p.m.	<b>1.1 SESSION KEYNOTE</b> Validation of Dietary Biomarkers in Multi-Ethnic Asian Population <i>Dorain Low, Nanyang Technological University, Singapore</i>	<b>165</b>
4:00 p.m. – 4:15 p.m.	<b>1.2</b> Lipidomic Studies Reveal Specific Circulating Phosphatidylcholines as Surrogate Biomarkers of Omega-3 Index <i>Philip Britz-McKibbin, McMaster University, Canada</i>	<b>302</b>
4:15 p.m. – 4:30 p.m.	<b>1.3</b> Metabolomics Identifies Molecular Pathways Linking Vitamin D to Allergic Airway Diseases in Childhood <i>Chih-Yung Chiu, Clinical Metabolomics Core Laboratory, Chang Gung Memorial Hospital at Linkou, Taiwan</i>	<b>120</b>
4:30 p.m. – 4:45 p.m.	<b>1.4</b> The effect of the 12 weeks replacement of animal-based proteins with plant ones on serum metabolite profiles in healthy adults ★ <i>Topi Meuronen, University Of Turku, Finland</i>	<b>291</b>
4:45 p.m. – 5:00 p.m.	<b>1.5</b> Assessing Adherence to Healthy Dietary Habits: the plasma nutrimental fingerprints in frail elderly <i>Laura Brunelli, Istituto Di Ricerche Farmacologiche Mario Negri Irccs, Italy</i>	<b>275</b>
5:00 p.m. – 5:15 p.m.	<b>1.6</b> Effects of Diets Varying in Carbohydrate and Fat on Metabolomics: A Randomized Controlled Feeding Study <i>Angeliki Angelidi, BCH; Harvard Medical School; Broad Institute of MIT and Harvard, United States</i>	<b>232</b>

## TECHNOLOGY ADVANCEMENTS

## COMPUTATIONAL METABOLOMICS, STATISTICS & BIOINFORMATICS

### ★ AWARD WINNERS

Monday, June 19		
Time	Session	Abstract #
<b>3:30 p.m. – 5:15 p.m.</b>	<b>Session 2. In-Depth and Real-Time Analysis</b> <i>Session Chairs: María Eugenia Monge and Roy Goodacre</i>	<b>Peller C</b>
3:30 p.m. – 4:00 p.m.	<b>2.1 KEYNOTE</b> Development of next generation metabolomics technologies for trans-omics <i>Takeshi Bamba, Kyushu University, Japan</i>	<b>346</b>
4:00 p.m. – 4:15 p.m.	<b>2.2</b> Fully Automated Metabolite Purification by Online-Micro-SPE-UPLC-MS <i>Gerd U. Balcke, Leibniz-Institute of Plant Biochemistry, Germany</i>	<b>194</b>
4:15 p.m. – 4:30 p.m.	<b>2.3</b> LC-IMS-MS vs LC-QTOF for comprehensive untargeted brain lipidomics <i>Maria Moran-Garrido, CEMBIO, Univ. San Pablo-CEU, Spain</i>	<b>277</b>
4:30 p.m. – 4:45 p.m.	<b>2.4</b> Unique chemoselective probes for discovery and investigation of metabolites in human samples with enhanced mass spectrometric sensitivity ★ <i>Weifeng Lin, Uppsala University, Sweden</i>	<b>148</b>
4:45 p.m. – 5:00 p.m.	<b>2.5</b> Intra- and Extracellular Metabolic Investigation of Perfused Fibroblasts by Real-time NMR Allows for Better Discrimination of Mitochondrial Defects ★ <i>Christian Urzi, University of Bern, Switzerland</i>	<b>169</b>
5:00 p.m. – 5:15 p.m.	<b>2.6</b> Environmental In-vivo NMR: Experiments, Instrumentation and the Introduction of Something a Little Special! <i>Andre Simpson, University of Toronto, Canada</i>	<b>244</b>
<b>3:30 p.m. – 5:15 p.m.</b>	<b>Session 3. Metabolite Annotation and Identification</b> <i>Session Chairs: Tao Huan and Eiichiro Fukusaki</i>	<b>Peller D</b>
3:30 p.m. – 4:00 p.m.	<b>3.1 KEYNOTE</b> Breaking Bonds & Barriers: Computational Metabolomics Strategies to Organize, Prioritize, and Annotate Metabolites in Mass Spectrometry Profiles <i>Justin JJ van der Hooft, Wageningen University &amp; Research, Netherlands</i>	<b>499</b>
4:00 p.m. – 4:15 p.m.	<b>3.2</b> CFM-ID 4 Plus: An Improved MS/MS Prediction Tool <i>Fei Wang, University Of Alberta, Canada</i>	<b>446</b>
4:15 p.m. – 4:30 p.m.	<b>3.3</b> Universal Fragmentation Model for Tandem Mass Spectrometry Based Molecular Structure Elucidation <i>Bela Paizs, Rosalind Franklin Institute/deShape Ltd., United Kingdom</i>	<b>319</b>
4:30 p.m. – 4:45 p.m.	<b>3.4</b> Towards a Rosetta stone for metabolomics: recommendations to overcome inconsistent metabolite nomenclature ★ <i>Ville Koistinen, University of Turku, Finland</i>	<b>215</b>
4:45 p.m. – 5:00 p.m.	<b>3.5</b> Chemical formulae as a unified representation for learning to generate and annotate mass spectra ★ <i>Samuel Goldman, MIT, United States</i>	<b>327</b>
5:00 p.m. – 5:15 p.m.	<b>3.6</b> Using Biotransformation Rules to Generate Novel Molecular Structures for Spectra Annotation in Molecular Network <i>Margaret Martin, Tufts University, United States</i>	<b>341</b>

## ★ AWARD WINNERS

Tuesday, June 20		
Time	Session	Abstract #
8:30 a.m. – 9:30 a.m.	<b>Plenary Session 2</b> Tracing Toxicants – Exposure Assessment for Environment and Health <i>Marja Lamoree, Vrije Universiteit, Amsterdam Institute for Life and Environment, Netherlands</i>	<i>Fallsview</i>
10:15 a.m. – 12:00 p.m.	<b>Session 4. Cardiovascular and Metabolic Diseases</b> <i>Session Chairs: Matej Orešič and Sandi Azab</i>	<i>Fallsview</i>
10:15 a.m. – 10:45 a.m.	<b>4.1 KEYNOTE</b> Ethnic variation and Metabolomic profiling of Gestational Diabetes and cardio-metabolic profiles of offspring <i>Sonia Anand, McMaster University, Canada</i>	<b>522</b>
10:45 a.m. – 11:00 a.m.	<b>4.2</b> Physiological Metabolomic Effects of a Cardiorenal Protective Diet Intervention in African Americans with Chronic Kidney Disease and Hypertension <i>Meera Patel, University of Texas Southwestern Medical Center, United States</i>	<b>162</b>
11:00 a.m. – 11:15 a.m.	<b>4.3</b> Role of human blood plasma metabolites in prediabetes and Type 2 Diabetes from IMI-DIRECT study <i>Sapna Sharma, Technical University Of Munich, Germany</i>	<b>129</b>
11:15 a.m. – 11:30 a.m.	<b>4.4</b> Investigation of lipid plasma profiles and microbiome composition during early stages of atherosclerosis induced by low carbohydrate – high protein diet in ApoE-knockout mice. <i>Lise Cougnaud, Concordia University, Canada</i>	<b>195</b>
11:30 a.m. – 11:45 a.m.	<b>4.5</b> Valvular Prostaglandins are Elevated with Human Aortic Valve Stenosis ★ <i>Lucien Cayer, University Of Manitoba, Canada</i>	<b>202</b>
11:45 a.m. – 12:00 p.m.	<b>4.6</b> Pathophysiological lipid changes in alcohol related liver disease <i>Kajetan Trošt, NNF Center for Basic Metabolic Research, University of Copenhagen, Denmark</i>	<b>207</b>

★ **AWARD WINNERS**

Tuesday, June 20		
Time	Session	Abstract #
<b>10:15 a.m. – 12:00 p.m.</b>	<b>Session 5. Novel Methods in Metabolomics</b> <i>Session Chairs: Dan Raftery and Meera Shanmuganathan</i>	<b>Peller C</b>
10:15 a.m. – 10:45 a.m.	<b>5.1 KEYNOTE</b> MS-based strategies for understanding clear cell Renal Cell Carcinoma, and new tools for data quality assessment in untargeted workflows <i>María Monge, Centro de Investigaciones en Bionanociencias (CIBION) – CONICET, Argentina</i>	<b>491</b>
10:45 a.m. – 11:00 a.m.	<b>5.2</b> Parallel Mass Spectrometric Investigation of Major Phase II Metabolite Classes in Human Samples <i>Ioanna Tsiara, Uppsala University, Sweden</i>	<b>321</b>
11:00 a.m. – 11:15 a.m.	<b>5.3</b> Finding Reactome pathways for MS disease severity based on proteomic and lipidomic signature enrichment: an Untargeted Integrated Omics approach <i>Faraz Rashid, Henry Ford Health Detroit, MI, United States</i>	<b>440</b>
11:15 a.m. – 11:30 a.m.	<b>5.4</b> Pre-analytics in clinical metabolomics studies: a database-driven web application for tailored plasma and serum sampling protocols <i>Lisa Hahnefeld, Fraunhofer Institute for Translational Medicine and Pharmacology ITMP, Germany</i>	<b>389</b>
11:30 a.m. – 11:45 a.m.	<b>5.5</b> Development and validation of a steroidomics methodology for non-invasive biomonitoring in wildlife <i>Tom Cools, Laboratory Of Integrative Metabolomics, Ghent University, Belgium</i>	<b>284</b>
11:45 a.m. – 12:00 p.m.	<b>5.6</b> Novel metabolic changes in tissue injury – potential treatment routes <i>Elizabeth Want, Imperial College London, United Kingdom</i>	<b>315</b>
<b>10:15 a.m. – 12:00 p.m.</b>	<b>Session 6. Non-targeted Analysis in Biomonitoring</b> <i>Session Chairs: Jonathan Mosley and Karl Jobst</i>	<b>Peller D</b>
10:15 a.m. – 10:45 a.m.	<b>6.1 KEYNOTE</b> Metabolomics in chemical and agrochemical industry: from development to registration <i>Hennicke Kamp, BASF Metabolome Solutions GmbH, Germany</i>	<b>502</b>
10:45 a.m. – 11:00 a.m.	<b>6.2</b> A multi-platform metabolomics, lipidomics and transcriptomics approach of the time and dose related effects of 6 model Metabolic Disrupting Chemicals under study in the GOLIATH EU H2020 project <i>Benedict Yanibada, UMR1331 Toxalim, Université de Toulouse, INRAE, France</i>	<b>403</b>
11:00 a.m. – 11:15 a.m.	<b>6.3</b> Perinatal exposure to endocrine disruptors: key learnings from metabolome mapping of rat models <i>Sara Evangelista, Vrije Universiteit, Netherlands</i>	<b>361</b>
11:15 a.m. – 11:30 a.m.	<b>6.4</b> Urban and Agriculture Impacts on River Estuaries in South Africa: Untargeted Tandem Mass Spectrometry as a Tool to Track Xenobiotic Dynamics <i>Jarmo-Charles Kalinski, Rhodes University, South Africa</i>	<b>441</b>
11:30 a.m. – 11:45 a.m.	<b>6.5</b> Disrupted lipid metabolism by PFHxS during different stages of early zebrafish development <i>Pim Leonards, Vrije Universiteit Amsterdam, Netherlands</i>	<b>362</b>
11:45 a.m. – 12:00 p.m.	<b>6.6</b> Unravelling the biological impact and metabolic burden of PFAS contamination in wild-caught freshwater turtles using omics-based ecosurveillance techniques. <i>David Beale, CSIRO, Australia</i>	<b>305</b>

## ★ AWARD WINNERS

Tuesday, June 20		
Time	Session	Abstract #
12:20 p.m. – 1:20 p.m.	<b>Sponsor Lunch Presentations</b>	
	<b>SCIEX</b> Busting Some Myths About Quantitative Metabolomics <i>David Wishart, Professor, Departments of Biological Sciences and Computing Science, University of Alberta</i>	<b>Fallsview</b>
	<b>Agilent Technologies</b> Next-Generation Metabolomics Analysis of Human Plasma Identifies Metabolites Associated with COVID-19 Severity <i>Ethan Stancliffe, Ph.D Student, Computational and Systems Biology, Washington University</i> Automation in Targeted Multi-omics Workflows <i>Dan Cuthbertson, Global Cell Biology &amp; Disease Research Segment Manager, Agilent Technologies</i> Future Trends in Metabolomics <i>Gary Patti, Ph.D, Professor, Departments of Chemistry, Genetics, and Medicine – Washington University; Chief Scientific Officer, PanomeBio</i>	<b>Peller C</b>
	<b>Metabolon</b> The Molecular Human – A Roadmap of Molecular Interactions Linking Multi-omics Networks with Disease Endpoints <i>Anna Halama, Assistant Professor of Research in Physiology and Biophysics, Weill Cornell Medicine Qatar</i>	<b>Peller D</b>
1:30 p.m. – 3:15 p.m.	<b>Session 7. Cancer</b> <i>Session Chairs: Daina Avizonis and Caroline Johnson</i>	<b>Fallsview</b>
1:30 p.m. – 1:50 p.m.	<b>7.1</b> Serum metabolome profiles in participants of the HUNT2 study were associated with long-term risk of breast cancer in an age-dependent manner <i>Karol Jelonek, Maria Sklodowska-Curie National Research Institute Of Oncology Gliwice Branch, Poland</i>	<b>168</b>
1:50 p.m. – 2:05 p.m.	<b>7.2</b> Discovery of decreased ferroptosis in male colorectal cancer patients with KRAS mutations <i>Hong Yan, Yale University, China</i>	<b>152</b>
2:05 p.m. – 2:25 p.m.	<b>7.3</b> Blood Metabolomic Profile of Glioma Risk: A Pooled, Multi-Cohort Analysis within COMETS <i>Demetrius Albanes, Division of Cancer Epidemiology and Genetics, National Cancer Institute, NIH, United States</i>	<b>182</b>
2:25 p.m. – 2:40 p.m.	<b>7.4</b> Preoperative Circulating 11-Oxygenated Androgens Are Associated with Metastasis-free Survival in Localized Prostate Cancer <i>Cylia Dahmani, Centre De Recherche Du Centre Hospitalier Universitaire De Québec, Canada</i>	<b>373</b>
2:40 p.m. – 3:00 p.m.	<b>7.5</b> Mapping of the Human Cell Metabolome Identifies Novel Cancer Therapeutic Targets in MYC-amplified Group 3 Medulloblastoma <i>J. Rafael Montenegro Burke, University Of Toronto, Canada</i>	<b>306</b>
3:00 p.m. – 3:15 p.m.	<b>7.6</b> From Operation Theater to Tissue-Multiomics Analysis – A Roadmap for Translational Cancer Research <i>Anna Halama, Weill Cornell Medicine Qatar, Qatar</i>	<b>397</b>

★ **AWARD WINNERS**

Tuesday, June 20		
Time	Session	Abstract #
<b>1:30 p.m. – 3:15 p.m.</b>	<b>Session 8. Multi-omics and Meta-analysis</b> <i>Session Chairs: Fabien Jourdan and Takeshi Bamba</i>	<b>Peller C</b>
1:30 p.m. – 1:50 p.m.	<b>8.1</b> COMETS Analytics and RaMP-DB to Enable Meta-Analyses of Metabolomic and Multi-Omic Data <i>Ewy Mathe, National Center For Advancing Translational Sciences, United States</i>	<b>394</b>
1:50 p.m. – 2:05 p.m.	<b>8.2</b> Pathway-based integration of metabolomics and multi-omics data using multivariate modelling approaches <i>Cecilia Wieder, Imperial College London, United Kingdom</i>	<b>172</b>
2:05 p.m. – 2:25 p.m.	<b>8.3</b> Integrative systems analysis-based risk stratification for immunometabolic complications in well-treated HIV-infected individuals <i>Ujjwal Neogi, Karolinska Institutet, Sweden</i>	<b>167</b>
2:25 p.m. – 2:40 p.m.	<b>8.4</b> Integrated transcriptome and metabolome analysis highlights the role of glycine, serine, and threonine metabolism in IgE levels in pediatric asthma <i>Tara Eicher, National Center For Advancing Translational Sciences, United States</i>	<b>375</b>
2:40 p.m. – 3:00 p.m.	<b>8.5</b> Linking metabolomics to genomics, microbiome and exposome – concepts, strategies, and platforms <i>Jianguo (Jeff) Xia, McGill University, Canada</i>	<b>343</b>
3:00 p.m. – 3:15 p.m.	<b>8.6</b> Untargeted metabolomics and transcriptomics uncover interspecies interactions in the soil microbiome <i>Francesco Del Carratore, University of Liverpool, United Kingdom</i>	<b>218</b>
<b>1:30 p.m. – 3:15 p.m.</b>	<b>Session 9. Foodomics and Food Security</b> <i>Session Chairs: David Liscombe and Jules Griffin</i>	<b>Peller D</b>
1:30 p.m. – 1:50 p.m.	<b>9.1</b> The Periodic Table of Food Initiative Enables Standardized Metabolomics for Global Food Analysis <i>Arpana Vaniya, UC Davis West Coast Metabolomics Center, United States</i>	<b>463</b>
1:50 p.m. – 2:05 p.m.	<b>9.2</b> LC-MS-based metabolomics to explore the phenolic profile of major and minor cereal crops ★ <i>Luciana Lima, Federal University of the State of Rio de Janeiro (UNIRIO), Brazil</i>	<b>411</b>
2:05 p.m. – 2:25 p.m.	<b>9.3</b> Metagenomic, metabolomic and sensorial characteristics of fermented Coffea arabica L. var. Castillo beans inoculated with microbial starter cultures <i>Mónica Cala, Universidad de Los Andes, Colombia</i>	<b>371</b>
2:25 p.m. – 2:40 p.m.	<b>9.4</b> Changes in edible insect metabolome after altering the feed composition by rapeseed meal ★ <i>Kateřina Šebelová, University Of Chemistry And Technology Prague, Czech Republic</i>	<b>294</b>
2:40 p.m. – 3:00 p.m.	<b>9.5</b> Untargeted metabolomic approaches for the search of common circulating metabolites coming from different bioactive plant extracts <i>Álvaro Fernández-Ochoa, University of Granada, Spain</i>	<b>222</b>
3:00 p.m. – 3:15 p.m.	<b>9.6</b> 1H NMR-based metabolomics combined with machine learning for the differentiation of varieties & detection of adulteration of Chinese oolong teas <i>Hui Ru Tan, National University Of Singapore, Singapore</i>	<b>102</b>



★ AWARD WINNERS

Tuesday, June 20				
Time	Session	Abstract #		
3:30 p.m. – 5:15 p.m.	<p><b>Session 10. Vendor Session</b> (Presented by Platinum and Gold sponsors) <i>Session Chairs: James Harynuk and Kati Hanhineva</i></p>	Fallsview		
3:30 p.m. – 4:25 p.m.	<p><b>PLATINUM PRESENTERS –</b></p> <p><b>Thermo Fisher Scientific</b> Susan S. Bird, Sr. Manager, Metabolomics and Lipidomics Team Lead, United States <b>Simultaneous Quantitation and Discovery (SQUAD) Metabolomics: Orbitrap based methods to empower your research</b></p> <hr/> <p><b>SCIEX</b> David Colquhoun, Market Development Manager, United States <b>ZenoTOF 7600: Technology Introduction</b></p> <hr/> <p><b>Bruker</b> Matthew R. Lewis PhD, FRSC, Director of Metabolomics Applications, United States <b>Unlock the Power of NMR and MS in Metabolomics: A Comprehensive Approach</b></p> <hr/> <p><b>Agilent Technologies</b> Dan Cuthbertson, Global Cell Biology &amp; Disease Research Segment Manager, United States <b>Agilent Solutions for Metabolomics Research</b></p> <hr/> <p><b>Metabolon</b> Dr. Annie Evans, Sr. Director, Head of Core Research, United States <b>Small Molecules, Big Insights – Delivering on the full potential of Metabolomics</b></p>			
	4:25 p.m. – 5:15 p.m.		<p><b>GOLD PRESENTERS –</b></p> <p><b>LECO Corporation</b> John Hayes, Separation Science Product Manager, United States <b>From Derivatization to Data Processing– Developing the Complete GC Metabolomics Solution</b></p> <hr/> <p><b>biocrates life sciences ag</b> Alice Limonciel, Senior Scientist   Scientific Storytelling, Austria <b>Quantitative Metabolomics Database (QMDB): Get access to reference ranges for 630 metabolites</b></p> <hr/> <p><b>Owlstone Medical</b> Dr Elizabeth Crone, Head of Business Development – Research Products and Services, United Kingdom <b>The ATLAS Project: Mapping Volatile Metabolites in Breath for Non-Invasive Biomarker Discovery</b></p> <hr/> <p><b>Cambridge Isotope Labs</b> Andrew Percy, PhD, Senior Applications Scientist, United States <b>Standard Isotopic Tools for QC and Quantification in MS Metabolomics</b></p> <hr/> <p><b>Miltenyi Biotec</b> Megan Ciarlo, Technology and Applications Specialist, United States <b>Realize authentic metabolomics data through gentle microfluidics cell sorting</b></p>	

# MENTAL HEALTH, DRUG ADDICTION AND MEDICINAL CANNABIS PLANTS, FOOD, ENVIRONMENT AND MICROBES

## ★ AWARD WINNERS

Tuesday, June 20		
Time	Session	Abstract #
<b>3:30 p.m. – 5:15 p.m.</b>	<b>Session 11. Neurological Disorders and Medicinal Cannabis</b> <i>Session Chairs: Rima Kaddurah-Daouk and Gabi Kastenmüller</i>	<b>Peller C</b>
3:30 p.m. – 4:00 p.m.	<b>11.1 KEYNOTE</b> Metabolomic approaches to exploring medicinal cannabis and the endocannabinidiome in health and disease <i>Scott Smid, The University Of Adelaide, Australia</i>	<b>501</b>
4:00 p.m. – 4:15 p.m.	<b>11.2</b> Linking Urinary Cannabinoid Metabolism with Behavioural and Neural Motivational Profiles of Cannabis Users <i>Iris Balodis, McMaster University, Canada</i>	<b>422</b>
4:15 p.m. – 4:30 p.m.	<b>11.3</b> Unraveling the metabolomic architecture of autism in a large Danish population-based cohort <i>Filip Ottosson, Statens Serum Institut, Denmark</i>	<b>363</b>
4:30 p.m. – 4:45 p.m.	<b>11.4</b> Integration of metabolomics research into translational clinical care: cerebrospinal fluid biomarkers for neuroinflammation ★ <i>Jinni Jingya Yan, Kids Neuroscience Centre, The Children's Hospital at Westmead, University of Sydney, Australia</i>	<b>236</b>
4:45 p.m. – 5:00 p.m.	<b>11.5</b> Baseline plasma metabolites predict cognitive decline after two years in the FINGER trial <i>Rui Climaco Pinto, Imperial College London, United Kingdom</i>	<b>450</b>
5:00 p.m. – 5:15 p.m.	<b>11.6</b> A multiomics approach to connect peripheral and central metabolism in Alzheimer's disease ★ <i>Nuanyi Liang, University Of California, Davis, United States</i>	<b>329</b>
<b>3:30 p.m. – 5:15 p.m.</b>	<b>Session 12. Microbial Metabolomics</b> <i>Session Chairs: Antonia García and Laura-Isobel McCall</i>	<b>Peller D</b>
3:30 p.m. – 4:00 p.m.	<b>12.1 KEYNOTE</b> Understanding the complexity of cacao spontaneous fermentation: applying integrated metabolomics, deep learning, and big data technologies. <i>Ian Castro-Gamboa, IQ-UNESP, Brazil</i>	<b>482</b>
4:00 p.m. – 4:15 p.m.	<b>12.2</b> Untargeted Metabolomic Profiling of Staphylococcus sp. Bridges the Gap between Metabolic and Genetic Variations ★ <i>Minghao Gong, The Jackson Laboratory for Genomic Medicine, United States</i>	<b>331</b>
4:15 p.m. – 4:30 p.m.	<b>12.3</b> A multi-omics approach toward reducing STI susceptibility in high-risk populations: The effects of intravaginal estrogen and/or probiotic interventions on the vaginal microenvironment <i>Biban Gill, McMaster University, Canada</i>	<b>451</b>
4:30 p.m. – 4:45 p.m.	<b>12.4</b> Spent media analysis and metabolic modelling of recombinant E. coli ★ <i>Hardik Dodia, Indian Institute of Technology Bombay, India</i>	<b>212</b>
4:45 p.m. – 5:00 p.m.	<b>12.5</b> Untargeted bacterial-metabolomics using ion-chromatography-mass spectrometry. <i>Kyoungeun Lee, University Of Oxford, United Kingdom</i>	<b>376</b>
5:00 p.m. – 5:15 p.m.	<b>12.6</b> Dynamic metabolic flux analysis during photosynthesis activation in cyanobacteria ★ <i>Kenya Tanaka, Kobe University, Japan</i>	<b>208</b>

## ★ AWARD WINNERS

Wednesday, June 21		
Time	Session	Abstract #
8:30 a.m. – 9:30 a.m.	<b>Plenary Session 3</b> Enhancing biological discovery in metabolomics through the use of stable isotopes <i>Gary Patti, Washington University, United States</i>	<i>Fallsview</i>
10:15 a.m. – 12:00 p.m.	<b>Session 13. Microbiome</b> <i>Session Chairs: Ian Lewis and Tom Metz</i>	<i>Fallsview</i>
10:15 a.m. – 10:35 a.m.	<b>13.1</b> A multi-omics approach reveals the uniqueness of the gut microbiota and fecal metabolome of young infants compared to their maternal lineage ★ <i>Tomás Clive Barker-Tejeda, CEMBIO, Universidad CEU San Pablo, Spain</i>	<b>296</b>
10:35 a.m. – 10:50 a.m.	<b>13.2</b> Integrating microbiome and metabolome data to understand effects of dietary interventions in multiple sclerosis <i>Friederike Gutmann, Max-Delbrück-Centrum für Molekulare Medizin, Germany</i>	<b>199</b>
10:50 a.m. – 11:10 a.m.	<b>13.3</b> Microbial metabolomics in human health and diseases, from in vitro to in vivo studies <i>Chris Zhu, The Ohio State University, United States</i>	<b>164</b>
11:10 a.m. – 11:25 a.m.	<b>13.4</b> Correlating human gut microbiota metabolites and composition in a longitudinal study ★ <i>Matteo Sangermani, NTNU, Norway</i>	<b>354</b>
11:25 a.m. – 11:45 a.m.	<b>13.5</b> Dynamics of Gut Metabolome and Microbiome Maturation during Early Life in the FinnBrain Birth Cohort Study <i>Alex Dickens, University Of Turku, Finland</i>	<b>444</b>
11:45 a.m. – 12:00 p.m.	<b>13.6</b> Brain Health at the Cross Roads of Genome Gut Microbiome Exposome and Metabolome <i>Rima Kaddurah-Daouk, Duke University, United States</i>	<b>457</b>

## ★ AWARD WINNERS

Wednesday, June 21		
Time	Session	Abstract #
<b>10:15 a.m. – 12:00 p.m.</b>	<b>Session 14. Reproducibility and QA/QC</b> <i>Session Chairs: Marcus Kim and Rick Dunn</i>	<b>Pager C</b>
10:15 a.m. – 10:35 a.m.	<b>14.1</b> Large-scale serum metabolome analyses by multisegment injection-capillary electrophoresis-mass spectrometry: Achieving high data fidelity with greater sample throughput for population health. <i>Zachary Kroezen, McMaster University, Canada</i>	<b>372</b>
10:35 a.m. – 10:50 a.m.	<b>14.2</b> QC procedure for untargeted LC-MS metabolomics for large-scale epidemiological studies <i>Mira Merdas, Nutrition And Metabolism Branch, International Agency For Research On Cancer (IARC), France</i>	<b>252</b>
10:50 a.m. – 11:10 a.m.	<b>14.3</b> mQACC: A community-led initiative to promote the development, dissemination and harmonization of best quality assurance and quality control practices and reporting in untargeted metabolomics research <i>Jonathan D. Mosley, US Environmental Protection Agency, United States</i>	<b>384</b>
11:10 a.m. – 11:25 a.m.	<b>14.4</b> Assessment of repeatability and reproducibility in untargeted LC/MS metabolomics: Beyond the limits of the relative standard deviation <i>Elfried B. M. Salanon, University of Clermont Auvergne, INRAE, UNH, Metabolism Exploration Platform, MetaboHUB, France</i>	<b>409</b>
11:25 a.m. – 11:45 a.m.	<b>14.5</b> Please, Tell Us What You Did: A literature review on the use of pooled quality control samples and associated disparity of reporting practices within the untargeted metabolomics community <i>Anne Evans, Metabolon, United States</i>	<b>443</b>
11:45 a.m. – 12:00 p.m.	<b>14.6</b> An Inter-laboratory study to investigate the use of 1D GC and 2D GCxGC -TOF-MS and -HRTOF-MS as Accurate, Robust, and Enriching Tools, for Non-targeted and Semi-targeted Analysis of Mammalian Biofluids <i>David Alonso, LECO Corporation, United States</i>	<b>434</b>

★ AWARD WINNERS

Wednesday, June 21		
Time	Session	Abstract #
<b>10:15 a.m. – 12:00 p.m.</b>	<b>Session 15. Ecosystem Metabolomics and Exposomics</b> <i>Session Chairs: Myrna Simpson and Hennieke Kamp</i>	<i>Peller D</i>
10:15 a.m. – 10:35 a.m.	<b>15.1</b> Demonstrating the reliability of metabolomics-based chemical grouping: Towards acceptable practice <i>Aniko Kende, Syngenta, United Kingdom</i>	<b>330</b>
10:35 a.m. – 10:50 a.m.	<b>15.2</b> An integrated molecular networking based non-targeted PFAS analysis workflow enables the identification of novel targets in NIST plasma. <i>Juan Moises Sanchez, Thermo Fisher Scientific, United States</i>	<b>147</b>
10:50 a.m. – 11:10 a.m.	<b>15.3</b> Novel biopesticide discovery using non-targeted metabolomics and plant-mediated RNAi for the lepidopteran pest management ★ <i>Manish Kumar, Indian Institute of Science Education and Research (IISER), India</i>	<b>224</b>
11:10 a.m. – 11:25 a.m.	<b>15.4</b> Acoustic and chemical impact of ship traffic on the metabolome of mussel larvae detected by NMR <i>Stephane Beauclercq, Université du Québec à Montréal, Canada</i>	<b>135</b>
11:25 a.m. – 11:45 a.m.	<b>15.5</b> Impact of in-utero exposures to perfluoroalkyl substances on the human fetal liver metabolome <i>Tuulia Hyötyläinen, Örebro University, Sweden</i>	<b>280</b>
11:45 a.m. – 12:00 p.m.	<b>15.6</b> Exposure to micro-/nanoplastics and the impact on early life development: a multi-omics approach <i>Lindsay Cahill, Memorial University of Newfoundland, Canada</i>	<b>380</b>
<b>12:20 p.m. – 1:20 p.m.</b>	<b>Sponsor Lunch Presentations</b>	
	<b>Thermo Fisher Scientific</b> Intelligent Metabolomics Workflows Powered by Orbitrap Technology <i>Rahul Deshpande, Marketing Specialist – Metabolomics, Thermo Fisher Scientific</i>	<i>Peller C</i>
	<b>Bruker Scientific</b> Decode Metabolomics: Unraveling Molecular Structures with NMR and Mass Spectrometry for Comprehensive Metabolome Profiling <i>Erica Forsberg, Global Director of Metabolomics, Bruker Scientific</i>	<i>Peller D</i>

## \*AWARD WINNERS

Wednesday, June 21		
Time	Session	Abstract #
<b>1:30 p.m. – 3:15 p.m.</b>	<b>Session 16. Epidemiology</b> <i>Session Chairs: Jessica Lasky-Su and Daniel Mutithu</i>	<i>Fallsview</i>
1:30 p.m. – 2:00 p.m.	<b>16.1 KEYNOTE</b> The Metabolomics of Mental Health Across the Lifecourse: a Spotlight on Tryptophan and Tyrosine metabolism <i>Rachel Kelly, Harvard Medical School, United States</i>	<b>503</b>
2:00 p.m. – 2:15 p.m.	<b>16.2</b> Plasma complex lipids in association with imaging markers of brain health: Findings from a population-based cohort study ★ <i>Elvire Landstra, German Centre for Neurodegenerative Diseases, Germany</i>	<b>226</b>
2:15 p.m. – 2:30 p.m.	<b>16.3</b> Development and validation of NMR metabolomic models of age and lifespan: A multi-cohort study <i>Chungho Lau, Imperial College London, United Kingdom</i>	<b>382</b>
2:30 p.m. – 2:45 p.m.	<b>16.4</b> A prospective study of whole blood trace element concentrations and pancreatic cancer in the Prostate, Lung, Colorectal and Ovarian Cancer Screening Trial Cohort <i>Rachael Stolzenberg-Solomon, DCEG, NCI, United States</i>	<b>175</b>
2:45 p.m. – 3:00 p.m.	<b>16.5</b> Demographic, Health, and Lifestyle Factors Associated with the Metabolome <i>Sandi Navarro, Fred Hutchinson Cancer Research Center, United States</i>	<b>123</b>
3:00 p.m. – 3:15 p.m.	<b>16.6</b> Using untargeted metabolomic profiling to provide robust prediction of a new biological aging phenotype derived from >30,000 patient electronic medical records <i>Qingwen Chen, Channing Division of Network Medicine, Brigham and Women's Hospital, United States</i>	<b>299</b>

## TECHNOLOGY ADVANCEMENTS

## PLANTS, FOOD, ENVIRONMENT AND MICROBES

### ★ AWARD WINNERS

Wednesday, June 21		
Time	Session	Abstract #
<b>1:30 p.m. – 3:15 p.m.</b>	<b>Session 17. New Advances in Lipidomics</b> <i>Session Chairs: Margret Thorsteinsdottir and Dajana Vuckovic</i>	<b>Peller C</b>
1:30 p.m. – 2:00 p.m.	<b>17.1 KEYNOTE</b> Lipidomics – the bumpy road of clinical translation <i>Anne Bendt, National University of Singapore, Singapore</i>	<b>507</b>
2:00 p.m. – 2:15 p.m.	<b>17.2</b> High-risk urine screening test for early detection of lysosphingolipidoses using a tandem mass spectrometry approach <i>Tristan Martineau, Université De Sherbrooke, Canada</i>	<b>228</b>
2:15 p.m. – 2:30 p.m.	<b>17.3</b> Complete structure elucidation of anionic lipids by a novel electron-activated dissociation mass spectrometry: Plasma electron-induced dissociation <i>Takashi Baba, Sciex, Canada</i>	<b>254</b>
2:30 p.m. – 2:45 p.m.	<b>17.4</b> Plasma Lipidomics using MS2 Data Demonstrates Enhanced Capabilities of Quantification for diaPASEF Method Development <i>Premy Shanthamoorthy, University of Toronto, Canada</i>	<b>464</b>
2:45 p.m. – 3:00 p.m.	<b>17.5</b> Insights into the comprehensive analysis of oxidized arachidonoyl-containing phosphatidylcholines using a structural library from Ion Mobility-Mass Spectrometry <i>Sandra M. Camunas-Alberca, CEMBio, Spain</i>	<b>374</b>
3:00 p.m. – 3:15 p.m.	<b>17.6</b> Ultraviolet photodissociation (UVPD) mass spectrometry for structural characterization of lipids in biological matrices on chromatographic time scales <i>Rahul Ravi Deshpande, Thermo Fisher Scientific, United States</i>	<b>432</b>
<b>1:30 p.m. – 3:15 p.m.</b>	<b>Session 18. Plant Metabolomics I</b> <i>Session Chairs: Susan Murch and Millena Barros Santos</i>	<b>Peller D</b>
1:30 p.m. – 2:00 p.m.	<b>18.1 KEYNOTE</b> Mining multi-omes to dissect the seed gene regulation and nutrient dynamics in cereal towards protein improvement <i>Subhra Chakraborty, National Institute Of Plant Genome Research, India</i>	<b>536</b>
2:00 p.m. – 2:15 p.m.	<b>18.2</b> Application of plant metabolomics to assess moss response to light stress during boreal forest regeneration <i>Grace Callahan, Western University, Canada</i>	<b>230</b>
2:15 p.m. – 2:30 p.m.	<b>18.3</b> SCL15 regulates seed dormancy by integration of circadian clock, hormones and cell-wall remodelling <i>Ming-Jun Gao, Agriculture and Agri-Food Canada, Canada</i>	<b>300</b>
2:30 p.m. – 2:45 p.m.	<b>18.4</b> Terpenoid chemotypes in <i>Tanacetum vulgare</i> vary on a large scale across Germany <i>Humay Rahimova, Research Unit Environmental Simulation, Helmholtz Munich, Germany</i>	<b>314</b>
2:45 p.m. – 3:00 p.m.	<b>18.5</b> I Can't Believe It's in vivo! Active in vivo Plant Volatolomics using TD-GC×GC-TOFMS <i>Paulina de la Mata, University of Alberta, Canada</i>	<b>429</b>
3:00 p.m. – 3:15 p.m.	<b>18.6</b> Characterizing inulin in plant products using matrix-assisted laser desorption/ionization magnetic resonance mass spectrometry (MALDI-MRMS) <i>Ruey Leng Loo, Murdoch University, Australia</i>	<b>213</b>

## ★ AWARD WINNERS

Wednesday, June 21		
Time	Session	Abstract #
<b>3:30 p.m. – 5:30 p.m.</b>	<b>Session 19. Lung and Respiratory Diseases</b> <i>Session Chairs: Rachel Kelly and Liang Li</i>	<i>Fallsview</i>
3:30 p.m. – 4:00 p.m.	<b>19.1 SESSION KEYNOTE</b> Molecular profiling of asthmatics identifies sub-phenotypes for application in precision respiratory medicine <i>Craig Wheelock, Karolinska Institute, Sweden</i>	<b>399</b>
4:00 p.m. – 4:15 p.m.	<b>19.2</b> A step towards precision medicine: metabolite ratios are strong predictors of asthma phenotypes <i>Yulu Chen, Brigham and Women's Hospital, United States</i>	<b>338</b>
4:15 p.m. – 4:30 p.m.	<b>19.3</b> Metabolic phenotyping of cannabis use demonstrates poorer chronic lung health outcomes <i>Sofina Begum, Harvard Medical School, United States</i>	<b>337</b>
4:30 p.m. – 4:45 p.m.	<b>19.4</b> Volatolomic approach to characterise oxidative stress at the molecular level using in vitro models <i>Thibaut Dejong, OBIACChem Lab, University of Liege, Belgium</i>	<b>142</b>
4:45 p.m. – 5:00 p.m.	<b>19.5</b> Unravelling COVID-19 Associated Metabolic Phenotypes in a Multisite Study <i>Mohammad Mehdi Banoei, University Of Calgary, Canada</i>	<b>410</b>
5:00 p.m. – 5:15 p.m.	<b>19.6</b> LiLA: A Lipid Lung Atlas Using a Reliable Lipid Annotation Workflow <i>Belén Fernández Requena, Fundación Universitaria San Pablo CEU, Spain</i>	<b>250</b>
5:15 p.m. – 5:30 p.m.	<b>19.7</b> Major energetic pathways and inflammation factors perturbed in valvular heart disease patients undergoing valve replacement ★ <i>Daniel Mutithu, Cape Heart Institute, University of Cape Town, South Africa</i>	<b>233</b>



## TECHNOLOGY ADVANCEMENTS

## COMPUTATIONAL METABOLOMICS, STATISTICS & BIOINFORMATICS

### ★ AWARD WINNERS

Wednesday, June 21		
Time	Session	Abstract #
<b>3:30 p.m. – 5:15 p.m.</b>	<b>Session 20. High-throughput and Spatial Metabolomics</b> <i>Session Chairs: Philip Britz-McKibbin and Coral Barbas</i>	<b>Peller C</b>
3:30 p.m. – 4:00 p.m.	<b>20.1 SESSION KEYNOTE</b> Population scale LC-MS metabolomics screening of 500,000 serum samples identifies novel biomarkers for cancer, cardiovascular, and liver diseases <i>Tomer Shlomi, Metasight Diagnostics LTD, Israel</i>	<b>115</b>
4:00 p.m. – 4:15 p.m.	<b>20.2</b> 10-second diagnosis of morphometric and molecular classes of central nervous system cancers using metabolic lipids with picosecond infrared laser mass spectrometry <i>Arash Zarrine-Afsar, Princess Margaret Hospital Cancer Centre; University of Toronto, Canada</i>	<b>309</b>
4:15 p.m. – 4:30 p.m.	<b>20.3</b> The advancement of SPC (Supramolecular Phospholipid Composite) as a biomarker of inflammation, cardiovascular risk, and its clinical applications. <i>Samantha Lodge, Murdoch University, Australia</i>	<b>273</b>
4:30 p.m. – 4:45 p.m.	<b>20.4</b> Spinal cord lipidomic remodeling across six mouse mutant strains monitored by mass spectrometry imaging <i>Rachel S. Pryce, Université de Montréal, Canada</i>	<b>449</b>
4:45 p.m. – 5:00 p.m.	<b>20.5</b> Differential localization of the structural isomers PGE2 and PGD2 at the site of pregnancy implantation <i>Rae Maeda, Kyoto University, Japan</i>	<b>185</b>
5:00 p.m. – 5:15 p.m.	<b>20.6</b> Visualizing the regional metabolic alteration in diabetic cardiomyopathy using mass spectrometry imaging <i>Zhonghua Wang, Minzu University Of China, Canada</i>	<b>173</b>
<b>3:30 p.m. – 5:15 p.m.</b>	<b>Session 21. Data Processing and Machine Learning</b> <i>Session Chairs: David Wishart and Justin van der Hooft</i>	<b>Peller D</b>
3:30 p.m. – 4:00 p.m.	<b>21.1 SESSION KEYNOTE</b> Streamlining mass spectrometry data processing and spectral library generation in MZmine 3 <i>Tomáš Pluskal, IOCB Prague, Czech Republic</i>	<b>266</b>
4:00 p.m. – 4:15 p.m.	<b>21.2</b> Applications of Disparate LC-MS Alignment and Data Analysis in Metabolomics <i>Hani Habra, NIST, United States</i>	<b>460</b>
4:15 p.m. – 4:30 p.m.	<b>21.3</b> ms-mint: Scalable metabolomics with Python <i>Soren Wacker, University of Calgary, Canada</i>	<b>118</b>
4:30 p.m. – 4:45 p.m.	<b>21.4</b> Development of a Machine Learning Strategy for Quantitative Non-targeted Lipidomics <i>Alexandria Van Grouw, Department of Chemistry &amp; Biochemistry, Georgia Institute Of Technology, United States</i>	<b>203</b>
4:45 p.m. – 5:00 p.m.	<b>21.5</b> microbeMASST: taxonomic-informed mass spectrometry search tool for bacteria and fungi ★ <i>Simone Zuffa, University of California San Diego, United States</i>	<b>156</b>
5:00 p.m. – 5:15 p.m.	<b>21.6</b> Reanalyzing mass spectrometry data to develop metabolome cartography database <i>Hiroshi Tsugawa, Tokyo University of Agriculture and Technology, Japan</i>	<b>316</b>

## ★ AWARD WINNERS

Thursday, June 22		
Time	Session	Abstract #
8:30 a.m. – 9:30 a.m.	<b>Plenary Session 4</b> Cannabis Metabolomics <i>Susan J. Murch, The University of British Columbia, Canada</i>	<i>Fallsview</i>
10:30 a.m. – 12:15 p.m.	<b>Session 22. Pregnancy, Maternal and Neonatal Health</b> <i>Session Chairs: Natasa Giallourou and Mónica Cala</i>	<i>Fallsview</i>
10:30 a.m. – 10:50 a.m.	<b>22.1</b> The metabolomic profiling way for the screening of fetal anomalies <i>Jacopo Troisi, Theoreo SRL – University of Salerno, Italy</i>	<b>138</b>
10:50 a.m. – 11:05 a.m.	<b>22.2</b> Early sex-dependent differences in metabolic profiles of overweight and adiposity in young children: a case-control study ★ <i>Sandi Azab, McMaster University, Canada</i>	<b>116</b>
11:05 a.m. – 11:25 a.m.	<b>22.3</b> Hair and cord blood exposome in pregnancy and their relationship with air pollution, dietary intake, gestational diabetes mellitus, and infant neurodevelopment ★ <i>Ting-li Han, The Second Affiliated Hospital of Chongqing Medical University, China</i>	<b>139</b>
11:25 a.m. – 11:40 a.m.	<b>22.4</b> Maternal exposure to nanoplastics alters brain metabolism in fetal and adolescent mice ★ <i>Nikita Harvey, Memorial University Of Newfoundland, Canada</i>	<b>307</b>
11:40 a.m. – 12:00 p.m.	<b>22.5</b> Application of a mass-spectrometry-based untargeted metabolomics workflow for probing prenatal alcohol exposure <i>Alicia DiBattista, Children's Hospital Of Eastern Ontario RI, Canada</i>	<b>417</b>
12:00 p.m. – 12:15 p.m.	<b>22.6</b> Infant Feeding Patterns, the Fecal Metabolome, and Neurodevelopmental Outcomes <i>Bridget Chalifour, University Of Colorado Boulder, United States</i>	<b>420</b>

★ AWARD WINNERS

Thursday, June 22		
Time	Session	Abstract #
<b>10:30 a.m. – 12:15 p.m.</b>	<b>Session 23. Plant Metabolomics II</b> <i>Session Chairs: Tomáš Pluskal and Álvaro Fernández-Ochoa</i>	<b>Peller C</b>
10:30 a.m. – 10:50 a.m.	<b>23.1</b> Metabolic reprogramming of barley in response to foliar application of the dichlorinated substitute of anthranilic acid: A priming agent or inducer of acquired resistance? <i>Claude Yasmine Hamany Djande, University Of Johannesburg, South Africa</i>	<b>274</b>
10:50 a.m. – 11:05 a.m.	<b>23.2</b> Metabolomics approach reveals insight into the trait between plant-beneficial and potentially antagonistic fungi <i>Prasath Balaji Sivaprakasam Padmanaban, Helmholtz Munich, Germany</i>	<b>353</b>
11:05 a.m. – 11:25 a.m.	<b>23.3</b> Holobiomics: A Metabolomics-Based Approach for Mapping Microbial Metabolic Activity and Taxonomy in the Holobiont <i>Paolo Bonini, oloBion, Spain</i>	<b>413</b>
11:25 a.m. – 11:40 a.m.	<b>23.4</b> Multi-omics approach for correlation analysis between pathogenic symptoms, microbes, and metabolome of <i>Neopyropia yezoensis</i> <i>Hyeon-Jeong Bae, Hankuk University of Foreign Studies, South Korea</i>	<b>249</b>
11:40 a.m. – 12:00 p.m.	<b>23.5</b> Untargeted metabolite profiling to elucidate rhizosphere and leaf metabolome changes of wheat cultivars ( <i>Triticum aestivum</i> L.) treated with the plant growth-promoting rhizobacteria <i>Paenibacillus alvei</i> (T22) and <i>Bacillus subtilis</i> ★ <i>Manamele Dannies Mashabela, University Of Johannesburg, South Africa</i>	<b>103</b>
12:00 p.m. – 12:15 p.m.	<b>23.6</b> Unravelling the Curse of the Biennial Bearing Cycle in Apple <i>Priyanka Reddy, Agriculture Victoria Research, Australia</i>	<b>340</b>

## ★ AWARD WINNERS

Thursday, June 22		
Time	Session	Abstract #
<b>10:30 a.m. – 12:15 p.m.</b>	<b>Session 24. Data Harmonization and Metabolic Networks</b> <i>Session Chairs: Sofina Begum and Tracey Schock</i>	<i>Peller D</i>
10:30 a.m. – 10:50 a.m.	<b>24.1</b> NIST SRM 1950 Beyond the Certificate of Analysis: mQACC Call to Provide Qualitative and Quantitative Data <i>Clay Davis, National Institute of Standards and Technology, United States</i>	<b>237</b>
10:50 a.m. – 11:05 a.m.	<b>24.2</b> Effects of Preanalytical Sample Collection and Handling on Comprehensive Metabolite Measurements in Human Urine Biospecimens <i>John Braisted, NCATS/NIH, United States</i>	<b>342</b>
11:05 a.m. – 11:25 a.m.	<b>24.3</b> Standardised metabolite annotation workflows for enhancing biological interpretation in metabolomic data repositories <i>Warwick Dunn, University Of Liverpool, United Kingdom</i>	<b>216</b>
11:25 a.m. – 11:40 a.m.	<b>24.4</b> Using spectral matching for evaluating the performance of LC-MS metabolomics methods <i>Francesc Puig Castellví, European Genomic Institutes for Diabetes, France</i>	<b>234</b>
11:40 a.m. – 12:00 p.m.	<b>24.5</b> Modeling Blood Metabolite Homeostasis Reduces Unexplained Variance and Reveals Basal Metabolism Levels and Network Relationships <i>Daniel Raftery, University Of Washington, United States</i>	<b>458</b>
12:00 p.m. – 12:15 p.m.	<b>24.6</b> An Atlas of the Relationship Between the Urinary and Plasma Metabolites: Implications for Precision Medicine ★ <i>Kevin Mendez, Harvard Medical School, United States</i>	<b>312</b>
<b>12:30 p.m. – 2:00 p.m.</b>	<b>Plenary Session 5 and Awards / Closing</b> Optimizing Patient Prognosis through Metabolomics Approaches <i>Caroline Johnson, Yale School of Public Health, United States</i>	<i>Fallsview</i>