



19th 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 A		
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.	Opening Ceremony and Plenary Session 1 Metabolomics for Nutrition Research <i>Lorraine Brennan, University College Dublin, Ireland</i>	<i>Fallsview</i>
3:30 p.m. – 5:15 p.m.	Session 1. Diet and Nutrition <i>Session Chairs:</i>	<i>Fallsview</i>
3:30 p.m. – 4:00 p.m.	1.1 SESSION KEYNOTE Validation of Dietary Biomarkers in Multi-Ethnic Asian Population <i>Dorain Low, Nanyang Technological University, Singapore</i>	165
4:00 p.m. – 4:15 p.m.	1.2 Lipidomic Studies Reveal Specific Circulating Phosphatidylcholines as Surrogate Biomarkers of Omega-3 Index <i>Philip Britz-McKibbin, McMaster University, Canada</i>	302
4:15 p.m. – 4:30 p.m.	1.3 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>	120
4:30 p.m. – 4:45 p.m.	1.4 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>	291
4:45 p.m. – 5:00 p.m.	1.5 Assessing Adherence to Healthy Dietary Habits: the plasma nutrimetabolomics fingerprints in frail elderly <i>Laura Brunelli, Istituto Di Ricerche Farmacologiche Mario Negri Irccs, Italy</i>	275
5:00 p.m. – 5:15 p.m.	1.6 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>	232

TECHNOLOGY ADVANCEMENTS

COMPUTATIONAL METABOLOMICS, STATISTICS & BIOINFORMATICS

★ AWARD WINNERS

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

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Tuesday, June 20		
Time	Session	Abstract #
8:30 a.m. – 9:30 a.m.	Plenary Session 2 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.	Session 4. Cardiovascular and Metabolic Diseases <i>Session Chairs:</i>	<i>Fallsview</i>
10:15 a.m. – 10:45 a.m.	4.1 KEYNOTE Ethnic variation and Metabolomic profiling of Gestational Diabetes and cardio-metabolic profiles of offspring <i>Sonia Anand, McMaster University, Canada</i>	522
10:45 a.m. – 11:00 a.m.	4.2 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>	233
11:00 a.m. – 11:15 a.m.	4.3 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>	129
11:15 a.m. – 11:30 a.m.	4.4 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>	195
11:30 a.m. – 11:45 a.m.	4.5 Valvular Prostaglandins are Elevated with Human Aortic Valve Stenosis ★ <i>Lucien Cayer, University Of Manitoba, Canada</i>	202
11:45 a.m. – 12:00 p.m.	4.6 Pathophysiological lipid changes in alcohol related liver disease <i>Kajetan Trošt, NNF Center for Basic Metabolic Research, University of Copenhagen, Denmark</i>	207

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Tuesday, June 20		
Time	Session	Abstract #
10:15 a.m. – 12:00 p.m.	Session 5. Novel Methods in Metabolomics <i>Session Chairs:</i>	Peller C
10:15 a.m. – 10:45 a.m.	5.1 KEYNOTE 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>	491
10:45 a.m. – 11:00 a.m.	5.2 Parallel Mass Spectrometric Investigation of Major Phase II Metabolite Classes in Human Samples <i>Ioanna Tsiara, Uppsala University, Sweden</i>	321
11:00 a.m. – 11:15 a.m.	5.3 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>	440
11:15 a.m. – 11:30 a.m.	5.4 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>	389
11:30 a.m. – 11:45 a.m.	5.5 Development and validation of a steroidomics methodology for non-invasive biomonitoring in wildlife <i>Tom Cools, Laboratory Of Integrative Metabolomics, Ghent University, Belgium</i>	284
11:45 a.m. – 12:00 p.m.	5.6 Novel metabolic changes in tissue injury – potential treatment routes <i>Elizabeth Want, Imperial College London, United Kingdom</i>	315
10:15 a.m. – 12:00 p.m.	Session 6. Non-targeted Analysis in Biomonitoring <i>Session Chairs:</i>	Peller D
10:15 a.m. – 10:45 a.m.	6.1 KEYNOTE Metabolomics in chemical and agrochemical industry: from development to registration <i>Hennicke Kamp, BASF Metabolome Solutions GmbH, Germany</i>	502
10:45 a.m. – 11:00 a.m.	6.2 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>	403
11:00 a.m. – 11:15 a.m.	6.3 Non-targeted detection of contaminants (and their possible metabolites) in groundwater <i>Mulatu Yohannes Nanusha, Aarhus University, Denmark</i>	109
11:15 a.m. – 11:30 a.m.	6.4 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>	441
11:30 a.m. – 11:45 a.m.	6.5 Disrupted lipid metabolism by PFHxS during different stages of early zebrafish development <i>Pim Leonards, Vrije Universiteit Amsterdam, Netherlands</i>	362
11:45 a.m. – 12:00 p.m.	6.6 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>	305

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Tuesday, June 20		
Time	Session	Abstract #
12:20 p.m. – 1:20 p.m.	Sponsor Lunch Presentations	
	SCIEX	Fallsview
	Agilent Technologies	Peller C
	Metabolon	Peller D
1:30 p.m. – 3:15 p.m.	Session 7. Cancer <i>Session Chairs:</i>	Fallsview
1:30 p.m. – 1:50 p.m.	7.1 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>	168
1:50 p.m. – 2:05 p.m.	7.2 Discovery of decreased ferroptosis in male colorectal cancer patients with KRAS mutations <i>Hong Yan, Yale University, China</i>	152
2:05 p.m. – 2:25 p.m.	7.3 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>	182
2:25 p.m. – 2:40 p.m.	7.4 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>	373
2:40 p.m. – 3:00 p.m.	7.5 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>	306
3:00 p.m. – 3:15 p.m.	7.6 From Operation Theater to Tissue-Multiomics Analysis – A Roadmap for Translational Cancer Research <i>Anna Halama, Weill Cornell Medicine Qatar, Qatar</i>	397

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Tuesday, June 20		
Time	Session	Abstract #
1:30 p.m. – 3:15 p.m.	Session 8. Multi-omics and Meta-analysis <i>Session Chairs:</i>	Peller C
1:30 p.m. – 1:50 p.m.	8.1 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>	394
1:50 p.m. – 2:05 p.m.	8.2 Pathway-based integration of metabolomics and multi-omics data using multivariate modelling approaches <i>Cecilia Wieder, Imperial College London, United Kingdom</i>	172
2:05 p.m. – 2:25 p.m.	8.3 Integrative systems analysis-based risk stratification for immunometabolic complications in well-treated HIV-infected individuals <i>Ujjwal Neogi, Karolinska Institutet, Sweden</i>	167
2:25 p.m. – 2:40 p.m.	8.4 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>	375
2:40 p.m. – 3:00 p.m.	8.5 Linking metabolomics to genomics, microbiome and exposome – concepts, strategies, and platforms <i>Jianguo (Jeff) Xia, McGill University, Canada</i>	343
3:00 p.m. – 3:15 p.m.	8.6 Untargeted metabolomics and transcriptomics uncover interspecies interactions in the soil microbiome <i>Francesco Del Carratore, University of Liverpool, United Kingdom</i>	218
1:30 p.m. – 3:15 p.m.	Session 9. Foodomics and Food Security <i>Session Chairs:</i>	Peller D
1:30 p.m. – 1:50 p.m.	9.1 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>	463
1:50 p.m. – 2:05 p.m.	9.2 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>	411
2:05 p.m. – 2:25 p.m.	9.3 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>	371
2:25 p.m. – 2:40 p.m.	9.4 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>	294
2:40 p.m. – 3:00 p.m.	9.5 Monitoring the metabolite changes in bean-to-bar chocolate processing <i>Sastia Prama Putri, Osaka University, Japan</i>	379
3:00 p.m. – 3:15 p.m.	9.6 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>	102

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Tuesday, June 20		
Time	Session	Abstract #
3:30 p.m. – 5:15 p.m.	Session 10. Vendor Session <i>Session Chairs:</i>	<i>Fallsview</i>
	PLATINUM PRESENTERS – Thermo Fisher Scientific SCIEX Bruker Agilent Technologies Metabolon	
	GOLD PRESENTERS – LECO Biocrates Life Sciences Owlstone Medical Ltd Cambridge Isotope Labs Miltenyi Biotec	

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

★ AWARD WINNERS

Tuesday, June 20		
Time	Session	Abstract #
3:30 p.m. – 5:15 p.m.	Session 11. Neurological Disorders and Medicinal Cannabis <i>Session Chairs:</i>	Peller C
3:30 p.m. – 4:00 p.m.	11.1 KEYNOTE Metabolomic approaches to exploring medicinal cannabis and the endocannabinidiome in health and disease <i>Scott Smid, The University Of Adelaide, Australia</i>	501
4:00 p.m. – 4:15 p.m.	11.2 Linking Urinary Cannabinoid Metabolism with Behavioural and Neural Motivational Profiles of Cannabis Users <i>Iris Balodis, McMaster University, Canada</i>	422
4:15 p.m. – 4:30 p.m.	11.3 Unraveling the metabolomic architecture of autism in a large Danish population-based cohort <i>Filip Ottosson, Statens Serum Institut, Denmark</i>	363
4:30 p.m. – 4:45 p.m.	11.4 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>	236
4:45 p.m. – 5:00 p.m.	11.5 Baseline plasma metabolites predict cognitive decline after two years in the FINGER trial <i>Rui Climaco Pinto, Imperial College London, United Kingdom</i>	450
5:00 p.m. – 5:15 p.m.	11.6 A multiomics approach to connect peripheral and central metabolism in Alzheimer's disease ★ <i>Nuanyi Liang, University Of California, Davis, United States</i>	329
3:30 p.m. – 5:15 p.m.	Session 12. Microbial Metabolomics <i>Session Chairs:</i>	Peller D
3:30 p.m. – 4:00 p.m.	12.1 KEYNOTE Understanding the complexity of cacao spontaneous fermentation: applying integrated metabolomics, deep learning, and big data technologies. <i>Ian Castro-Gamboa, IQ-UNESP, Brazil</i>	482
4:00 p.m. – 4:15 p.m.	12.2 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>	331
4:15 p.m. – 4:30 p.m.	12.3 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>	451
4:30 p.m. – 4:45 p.m.	12.4 Spent media analysis and metabolic modelling of recombinant E. coli ★ <i>Hardik Dodia, Indian Institute of Technology Bombay, India</i>	212
4:45 p.m. – 5:00 p.m.	12.5 Untargeted bacterial-metabolomics using ion-chromatography-mass spectrometry. <i>Kyoungeun Lee, University Of Oxford, United Kingdom</i>	376
5:00 p.m. – 5:15 p.m.	12.6 Dynamic metabolic flux analysis during photosynthesis activation in cyanobacteria ★ <i>Kenya Tanaka, Kobe University, Japan</i>	208

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Wednesday, June 21		
Time	Session	Abstract #
8:30 a.m. – 9:30 a.m.	Plenary Session 3 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.	Session 13. Microbiome <i>Session Chairs:</i>	<i>Fallsview</i>
10:15 a.m. – 10:35 a.m.	13.1 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>	296
10:35 a.m. – 10:50 a.m.	13.2 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>	199
10:50 a.m. – 11:10 a.m.	13.3 Microbial metabolomics in human health and diseases, from in vitro to in vivo studies <i>Chris Zhu, The Ohio State University, United States</i>	164
11:10 a.m. – 11:25 a.m.	13.4 Correlating human gut microbiota metabolites and composition in a longitudinal study ★ <i>Matteo Sangermani, NTNU, Norway</i>	354
11:25 a.m. – 11:45 a.m.	13.5 Dynamics of Gut Metabolome and Microbiome Maturation during Early Life in the FinnBrain Birth Cohort Study <i>Alex Dickens, University Of Turku, Finland</i>	444
11:45 a.m. – 12:00 p.m.	13.6 Brain Health at the Cross Roads of Genome Gut Microbiome Exposome and Metabolome <i>Rima Kaddurah-Daouk, Duke University, United States</i>	457

★ AWARD WINNERS

Wednesday, June 21		
Time	Session	Abstract #
10:15 a.m. – 12:00 p.m.	Session 14. Reproducibility and QA/QC <i>Session Chairs:</i>	<i>Peller C</i>
10:15 a.m. – 10:35 a.m.	14.1 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>	372
10:35 a.m. – 10:50 a.m.	14.2 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>	252
10:50 a.m. – 11:10 a.m.	14.3 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>	384
11:10 a.m. – 11:25 a.m.	14.4 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, NIRAE, UNH, Metabolism Exploration Platform, MetaboHUB, France</i>	409
11:25 a.m. – 11:45 a.m.	14.5 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>	443
11:45 a.m. – 12:00 p.m.	14.6 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>	434

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Wednesday, June 21		
Time	Session	Abstract #
10:15 a.m. – 12:00 p.m.	Session 15. Ecosystem Metabolomics and Exposomics <i>Session Chairs:</i>	<i>Peller D</i>
10:15 a.m. – 10:35 a.m.	15.1 Demonstrating the reliability of metabolomics-based chemical grouping: Towards acceptable practice <i>Aniko Kende, Syngenta, United Kingdom</i>	330
10:35 a.m. – 10:50 a.m.	15.2 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>	147
10:50 a.m. – 11:10 a.m.	15.3 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>	224
11:10 a.m. – 11:25 a.m.	15.4 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>	135
11:25 a.m. – 11:45 a.m.	15.5 Impact of in-utero exposures to perfluoroalkyl substances on the human fetal liver metabolome <i>Tuulia Hyötyläinen, Örebro University, Sweden</i>	280
11:45 a.m. – 12:00 p.m.	15.6 Exposure to micro-/nanoplastics and the impact on early life development: a multi-omics approach <i>Lindsay Cahill, Memorial University of Newfoundland, Canada</i>	380
12:20 p.m. – 1:20 p.m.	Sponsor Lunch Presentations	
	Thermo Fisher Scientific	<i>Peller C</i>
	Bruker Scientific	<i>Peller D</i>

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Wednesday, June 21		
Time	Session	Abstract #
1:30 p.m. – 3:15 p.m.	Session 16. Epidemiology <i>Session Chairs:</i>	<i>Fallsview</i>
1:30 p.m. – 2:00 p.m.	16.1 KEYNOTE The Metabolomics of Mental Health Across the Lifecourse: a Spotlight on Tryptophan and Tyrosine metabolism <i>Rachel Kelly, Harvard Medical School, United States</i>	503
2:00 p.m. – 2:15 p.m.	16.2 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>	226
2:15 p.m. – 2:30 p.m.	16.3 Development and validation of NMR metabolomic models of age and lifespan: A multi-cohort study <i>Chungho Lau, Imperial College London, United Kingdom</i>	382
2:30 p.m. – 2:45 p.m.	16.4 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>	175
2:45 p.m. – 3:00 p.m.	16.5 Demographic, Health, and Lifestyle Factors Associated with the Metabolome <i>Sandi Navarro, Fred Hutchinson Cancer Research Center, United States</i>	123
3:00 p.m. – 3:15 p.m.	16.6 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>	299

TECHNOLOGY ADVANCEMENTS

PLANTS, FOOD, ENVIRONMENT AND MICROBES

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Wednesday, June 21		
Time	Session	Abstract #
1:30 p.m. – 3:15 p.m.	Session 17. New Advances in Lipidomics <i>Session Chairs:</i>	Peller C
1:30 p.m. – 2:00 p.m.	17.1 KEYNOTE Lipidomics – the bumpy road of clinical translation <i>Anne Bendt, National University of Singapore, Singapore</i>	507
2:00 p.m. – 2:15 p.m.	17.2 High-risk urine screening test for early detection of lysosphingolipidoses using a tandem mass spectrometry approach <i>Tristan Martineau, Université De Sherbrooke, Canada</i>	228
2:15 p.m. – 2:30 p.m.	17.3 Complete structure elucidation of anionic lipids by a novel electron-activated dissociation mass spectrometry: Plasma electron-induced dissociation <i>Takashi Baba, Sciex, Canada</i>	254
2:30 p.m. – 2:45 p.m.	17.4 Plasma Lipidomics using MS2 Data Demonstrates Enhanced Capabilities of Quantification for diaPASEF Method Development <i>Premy Shanthamoorthy, University of Toronto, Canada</i>	464
2:45 p.m. – 3:00 p.m.	17.5 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>	374
3:00 p.m. – 3:15 p.m.	17.6 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>	432
1:30 p.m. – 3:15 p.m.	Session 18. Plant Metabolomics I <i>Session Chairs:</i>	Peller D
1:30 p.m. – 2:00 p.m.	18.1 KEYNOTE 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>	536
2:00 p.m. – 2:15 p.m.	18.2 Metabolomics applications in plant sciences: elucidating modes of action of biostimulants <i>Fidele Tugizimana, University Of Johannesburg & Omnia Group Ltd, South Africa</i>	196
2:15 p.m. – 2:30 p.m.	18.3 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>	300
2:30 p.m. – 2:45 p.m.	18.4 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>	314
2:45 p.m. – 3:00 p.m.	18.5 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>	429
3:00 p.m. – 3:15 p.m.	18.6 Mass spectrometry-based metabolomics reveals the exchange of metabolites between neighboring plants ★ <i>Hossein Hazrati, Aarhus University, Denmark</i>	248

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Wednesday, June 21		
Time	Session	Abstract #
3:30 p.m. – 5:15 p.m.	Session 19. Lung and Respiratory Diseases <i>Session Chairs:</i>	<i>Fallsview</i>
3:30 p.m. – 4:00 p.m.	19.1 SESSION KEYNOTE Molecular profiling of asthmatics identifies sub-phenotypes for application in precision respiratory medicine <i>Craig Wheelock, Karolinska Institute, Sweden</i>	399
4:00 p.m. – 4:15 p.m.	19.2 A step towards precision medicine: metabolite ratios are strong predictors of asthma phenotypes <i>Yulu Chen, Brigham and Women's Hospital, United States</i>	338
4:15 p.m. – 4:30 p.m.	19.3 Metabolic phenotyping of cannabis use demonstrates poorer chronic lung health outcomes <i>Sofina Begum, Harvard Medical School, United States</i>	337
4:30 p.m. – 4:45 p.m.	19.4 Volatolomic approach to characterise oxidative stress at the molecular level using in vitro models <i>Thibaut Dejong, OBIACChem Lab, University of Liege, Belgium</i>	142
4:45 p.m. – 5:00 p.m.	19.5 Unravelling COVID-19 Associated Metabolic Phenotypes in a Multisite Study <i>Mohammad Mehdi Banoei, University Of Calgary, Canada</i>	410
5:00 p.m. – 5:15 p.m.	19.6 LiLA: A Lipid Lung Atlas Using a Reliable Lipid Annotation Workflow <i>Belén Fernández Requena, Fundación Universitaria San Pablo CEU, Spain</i>	250
3:30 p.m. – 5:15 p.m.	Session 20. High-throughput and Spatial Metabolomics <i>Session Chairs:</i>	<i>Peller C</i>
3:30 p.m. – 4:00 p.m.	20.1 SESSION KEYNOTE 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>	115
4:00 p.m. – 4:15 p.m.	20.2 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>	309
4:15 p.m. – 4:30 p.m.	20.3 The advancement of SPC (Supramolecular Phospholipid Composite) as a biomarker of inflammation, cardiovascular risk, and it's clinical applications. <i>Samantha Lodge, Murdoch University, Australia</i>	273
4:30 p.m. – 4:45 p.m.	20.4 An automated online three-phase electro-extraction setup with machine-vision process monitoring hyphenated to LC-MS analysis <i>Yupeng He, Leiden University, Netherlands</i>	197
4:45 p.m. – 5:00 p.m.	20.5 Differential localization of the structural isomers PGE2 and PGD2 at the site of pregnancy implantation <i>Rae Maeda, Kyoto University, Japan</i>	185
5:00 p.m. – 5:15 p.m.	20.6 Visualizing the regional metabolic alteration in diabetic cardiomyopathy using mass spectrometry imaging <i>Zhonghua Wang, Minzu University Of China, Canada</i>	173

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Wednesday, June 21		
Time	Session	Abstract #
3:30 p.m. – 5:15 p.m.	Session 21. Data Processing and Machine Learning <i>Session Chairs:</i>	<i>Peller D</i>
3:30 p.m. – 4:00 p.m.	21.1 SESSION KEYNOTE Streamlining mass spectrometry data processing and spectral library generation in MZmine 3 <i>Tomáš Pluskal, IOCB Prague, Czech Republic</i>	266
4:00 p.m. – 4:15 p.m.	21.2 Applications of Disparate LC-MS Alignment and Data Analysis in Metabolomics <i>Hani Habra, NIST, United States</i>	460
4:15 p.m. – 4:30 p.m.	21.3 ms-mint: Scalable metabolomics with Python <i>Soren Wacker, University of Calgary, Canada</i>	118
4:30 p.m. – 4:45 p.m.	21.4 Development of a Machine Learning Strategy for Quantitative Non-targeted Lipidomics <i>Alexandria Van Grouw, Department of Chemistry & Biochemistry, Georgia Institute Of Technology, United States</i>	203
4:45 p.m. – 5:00 p.m.	21.5 microbeMASST: taxonomic-informed mass spectrometry search tool for bacteria and fungi ★ <i>Simone Zuffa, University of California San Diego, United States</i>	156
5:00 p.m. – 5:15 p.m.	21.6 Reanalyzing mass spectrometry data to develop metabolome cartography database <i>Hiroshi Tsugawa, Tokyo University of Agriculture and Technology, Japan</i>	316

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Thursday, June 22		
Time	Session	Abstract #
8:30 a.m. – 9:30 a.m.	Plenary Session 4 Cannabis Metabolomics <i>Susan J. Murch, The University of British Columbia, Canada</i>	<i>Fallsview</i>
10:30 a.m. – 12:15 p.m.	Session 22. Pregnancy, Maternal and Neonatal Health <i>Session Chairs:</i>	<i>Fallsview</i>
10:30 a.m. – 10:50 a.m.	22.1 The metabolomic profiling way for the screening of fetal anomalies <i>Jacopo Troisi, Theoreo SRL – University of Salerno, Italy</i>	138
10:50 a.m. – 11:05 a.m.	22.2 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>	116
11:05 a.m. – 11:25 a.m.	22.3 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>	139
11:25 a.m. – 11:40 a.m.	22.4 Maternal exposure to nanoplastics alters brain metabolism in fetal and adolescent mice ★ <i>Nikita Harvey, Memorial University Of Newfoundland, Canada</i>	307
11:40 a.m. – 12:00 p.m.	22.5 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>	417
12:00 p.m. – 12:15 p.m.	22.6 Infant Feeding Patterns, the Fecal Metabolome, and Neurodevelopmental Outcomes <i>Bridget Chalifour, University Of Colorado Boulder, United States</i>	420

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Thursday, June 22		
Time	Session	Abstract #
10:30 a.m. – 12:15 p.m.	Session 23. Plant Metabolomics II <i>Session Chairs:</i>	Peller C
10:30 a.m. – 10:50 a.m.	23.1 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>	274
10:50 a.m. – 11:05 a.m.	23.2 Metabolomics approach reveals insight into the trait between plant-beneficial and potentially antagonistic fungi <i>Prasath Balaji Sivaprakasam Padmanaban, Helmholtz Munich, Germany</i>	353
11:05 a.m. – 11:25 a.m.	23.3 Holobiomics: A Metabolomics-Based Approach for Mapping Microbial Metabolic Activity and Taxonomy in the Holobiont <i>Paolo Bonini, oloBion, Spain</i>	413
11:25 a.m. – 11:40 a.m.	23.4 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>	249
11:40 a.m. – 12:00 p.m.	23.5 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>	103
12:00 p.m. – 12:15 p.m.	23.6 Unravelling the Curse of the Biennial Bearing Cycle in Apple <i>Priyanka Reddy, Agriculture Victoria Research, Australia</i>	340

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