



22nd Annual Conference of the Metabolomics Society

METABOLOMICS 2026

BUENOS AIRES ARGENTINA | JUNE 21-24



SCHEDULE OF
ORAL PRESENTATIONS

AGENDA AT A GLANCE

■ Metabolomics in Health and Disease
 ■ Technology Advancements
 ■ Computational Metabolomics, Statistics & Bioinformatics
 ■ Plants, Food, Environment and Microbes

SUNDAY, JUNE 21				
	Salon C1	Salon C2	Salon E	VIP2
7:30 a.m.	REGISTRATION / INFO DESK OPEN			
8:15 a.m. – 10:15 a.m.	W1: Cross-repository analysis of public met data w/ MetabolomicsHub	W2: Demystifying Stable Isotope Labelling Metabolomics	W3: LC-MS Data Processing with mzmine	
10:15 a.m. – 10:30 a.m.	COFFEE BREAK			
10:30 a.m. – 12:30 p.m.	W4: Metabolomics and AI Approaches for Precision Health	W5: CHESS-Hub and Mapping Community Needs in Metabolite ID	W6: MetaboApps in GNPS2	
12:30 p.m. – 1:30 p.m.	LUNCH – TICKET FOR PURCHASE			
1:30 p.m. – 3:30 p.m.	W7: EMN Career Development	W8: Quality Control in untargeted met using mQACC	W9: Introduction to MetExplore 3	W10: Multisegment Injection-Capillary Electrophoresis-Mass Spec
3:45 p.m. – 5:15 p.m.	Opening Ceremony & Plenary Session 1: Jessica Lasky-Su			
5:15 p.m. – 7:30 p.m.	Poster Session 1 & Welcome Reception (Poster Presentations from 5:15pm – 6:15pm)			
6:45 p.m. – 8:00 p.m.	Career Night Roundtable Discussions			
MONDAY, JUNE 22				
	Salon E	Salon C1	Salon C2	
8:00 a.m.	REGISTRATION / INFO DESK OPEN			
8:30 a.m. – 9:30 a.m.	Plenary Session 2 – Marta Cascante			
9:30 a.m. – 10:15 a.m.	COFFEE BREAK			
10:15 a.m. – 12:00 p.m.	1 Cardiometabolic & Organ-Specific Disease	2 Metabolite Annotation	3 Plants	
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: Shimadzu do Brasil Comercio	
1:30 p.m. – 3:00 p.m.	4 Multi-Omics	5 Standardization and Multi-Site Validation	6 Microorganisms	
3:00 p.m. – 3:30 p.m.	COFFEE BREAK			
3:30 p.m. – 5:15 p.m.	7 Neurological Disorders	8 Analytical Methods and Workflow Innovations	9 Food	
5:15 p.m. – 6:30 p.m.	Poster Session 2			
6:30 p.m. – 8:00 p.m.	EMN Reception			
TUESDAY, JUNE 23				
	Salon E	Salon C1	Salon C2	
8:15 a.m.	REGISTRATION / INFO DESK OPEN			
8:30 a.m. – 9:30 a.m.	Plenary Session 3 – Huiru Tang			
9:30 a.m. – 10:15 a.m.	COFFEE BREAK			
10:15 a.m. – 12:00 p.m.	10 Microbiota & Infectious Disease	11 Machine Learning and AI Systems	12 Ion Mobility and Integrated Workflows	
12:00 p.m. – 1:30 p.m.	LUNCH BREAK AND SPONSOR PRESENTATIONS			
12:20 p.m. – 1:20 p.m.	Sponsor Pres: Agilent Technologies	Sponsor Pres: Bruker	Sponsor Pres: Thermo Fisher Scientific	
1:30 p.m. – 3:00 p.m.	13 Immunometabolism and Infectious Disease	14 Real-Time Analysis	15 Plants and Food	
3:00 p.m. – 3:30 p.m.	COFFEE BREAK			
3:30 p.m. – 5:15 p.m.	16 Chemical Exposures and Bioactive Metabolites	17 Data Ecosystems and Knowledge Sharing	18 Environment I	
5:15 p.m. – 6:30 p.m.	Poster Session 3			
6:30 p.m. – 8:00 p.m.	Tango Social & Celebration			
WEDNESDAY, JUNE 24				
	Salon E	Salon C1	Salon C2	
9:00 a.m.	INFO DESK OPEN			
9:30 a.m. – 10:30 a.m.	Plenary Session 4 – Fidele Tugizimana			
10:30 a.m.– 11:30 a.m.	Poster Session 4			
11:30 a.m. – 1:15 p.m.	19 Environment II	20 Cancer Metabolomics	21 Nutrimetabolomics	
1:15 p.m. – 2:45 p.m.	LUNCH AND TOWN HALL MEETING			
1:35 p.m. – 2:35 p.m.	Town Hall Meeting			
2:45 p.m. – 4:30 p.m.	Plenary Session 5 – Mariana Larraz Ferreira – Awards and Closing			

★ AWARD WINNERS

Sunday, June 21		
Time	Session	Abstract #
3:45 p.m. – 5:15 p.m.	Opening Ceremony & Plenary Session 1 <i>Jessica Lasky-Su, Brigham & Women's Hospital, Harvard Medical School, United States</i> *Recipient of 2025 Metabolomics Society Honorary Fellowship From Discovery to Decision: How Integrative Metabolomics is Enabling Precision Medicine	Salon E

Monday, June 22		
Time	Session	Abstract #
8:30 a.m. – 9:30 a.m.	Plenary Session 2 <i>Marta Cascante, University of Barcelona, Spain</i> *Recipient of 2025 Metabolomics Society Honorary Fellowship From ¹³ C based metabolic flux analysis to genome scale metabolic modelling: identifying therapeutic vulnerabilities in cancer and multifactorial diseases	Salon E
10:15 a.m. – 12:00 p.m.	Session 1. Cardiometabolic & Organ-Specific Disease <i>Session Chairs: Julia Kuligowski & Nicholas Ratray</i>	Salon E
10:15 a.m. – 10:45 a.m.	1.1 KEYNOTE The Hidden Language of the Liver: Decoding Metabolic Secrets through Targeted and Untargeted Metabolomics and Lipidomics <i>Antonia Garcia, CEMBIO, Universidad San Pablo-CEU, Spain</i>	351
10:45 a.m. – 11:05 a.m.	1.2 Metabolomics Identifies Environmental Chemical Signatures of Steatotic Liver Disease with PFAS as Key Contributors <i>Tuulia Hyötyläinen, Orebro University, Sweden</i>	240
11:05 a.m. – 11:20 a.m.	1.3 Metabolomic ageing clock monitors risks of cardiometabolic diseases ★ Manyi Jia, Imperial College London, United Kingdom	53
11:20 a.m. – 11:40 a.m.	1.4 The Metabolomic Signature of Subclinical Atherosclerosis <i>Alessia Ferrarini, CNIC – Spanish National Center for Cardiovascular Research, Spain</i>	116
11:40 a.m. – 12:00 p.m.	1.5 When Heart Failure Mortality Presents as Metabolic: Metabolomic Signatures Predict 2-Year Mortalities Across Asia and Oceania ★ Lik Hang Wu, Kitasato University, Japan	56

★ **AWARD WINNERS**

Monday, June 22		
Time	Session	Abstract #
10:15 a.m. – 12:00 p.m.	Session 2. Metabolite Annotation <i>Session Chairs: Fabien Jourdan & Luciana Lima</i>	Salon C1
10:15 a.m. – 10:45 a.m.	2.1 KEYNOTE Prospecting bioactive compounds in microorganisms through omics data mining and innovative validation platforms <i>Ricardo da Silva, University of São Paulo, Brazil</i>	347
10:45 a.m. – 11:05 a.m.	2.2 Benchmarking an ion mobility–resolved LC–MS/MS library against GNPS highlights the importance of instrument-specific spectral libraries <i>Aninda Mazumdar, Mikrobiologicky ustav AV CR, Czech Republic</i>	272
11:05 a.m. – 11:20 a.m.	2.3 CASMI 2026: a real-world small molecule structure elucidation challenge, featuring hundreds of biologically-sourced challenge molecules (including many with novel structures) and the largest open-sourced library of novel small molecule LC-MS/MS spectra ever released <i>David Healey, Enveda, United States</i>	128
11:20 a.m. – 11:40 a.m.	2.4 Extending CEU Mass Mediator for Multi-Platform Metabolite Annotation in LC-MS, CE-MS and GC-MS <i>Alberto Gil-de-la-Fuente, CEU-san Pablo University, Spain</i>	172
11:40 a.m. – 12:00 p.m.	2.5 FLARE: Fine-grained Learning for Alignment of spectra-molecule REpresentation Enhances Metabolite Annotation ★ <i>Yan Zhou Chen, Tufts University, United States</i>	40
10:15 a.m. – 12:00 p.m.	Session 3. Plants <i>Session Chairs: Norberto Peporine Lopes & Paula Burdisso</i>	Salon C2
10:15 a.m. – 10:45 a.m.	3.1 KEYNOTE From UHPLC-MS Metabolomics to Metal Protection: Cinnamic Acid Derivatives as Green Corrosion Inhibitors <i>Edwin Madala, University of Venda, South Africa</i>	354
10:45 a.m. – 11:05 a.m.	3.2 Integrating metabolomics and MALDI-MS imaging reveals the efficacy of a novel elicitation strategy to induce spatially resolved chemical defenses in Eucalyptus. <i>Andy J. Pérez, Universidad De Concepcion, Chile</i>	294
11:05 a.m. – 11:20 a.m.	3.3 The Metabolic Awakening of Barley Seedlings: A Time-Resolved View of how Germination Shapes Tissue-Specific Metabolic Networks ★ <i>Claude Yasmine Hamany Djande, University Of Johannesburg, South Africa</i>	120
11:20 a.m. – 11:40 a.m.	3.4 Metabolic crosstalk between foliar metabolism and BVOC emissions reveals seasonal plasticity in an urban Atlantic Forest tree ★ <i>Fernanda Anselmo-Moreira, Environmental Research Institute (IPA-SP), Brazil</i>	77
11:40 a.m. – 12:00 p.m.	3.5 Two generations, two carbon economies: the hornwort sporophyte enriches shikimate and the TCA cycle <i>Ivan Hurtado Caceres, University of São Paulo, Brazil</i>	148

★ AWARD WINNERS

Monday, June 22		
Time	Session	Abstract #
12:20 p.m. – 1:20 p.m.	Sponsor Lunch Presentations	
	SCIEX Is your workflow giving you answers or just data? Integrating high-sensitivity exposomics and broad coverage metabolomics. <i>Vinicius Verri Hernandez, Senior Scientist, University of Vienna, Austria</i> ZT Scan DIA 3.0 across scales <i>Nicola Zamboni, Adjunct Professor, Institute of Molecular Systems Biology, ETH Zurich</i>	Salon C1
	Shimadzu do Brasil Comercio WHEN YOU KNOW WHAT THE ANSWER IS OUR EXPERIENCE WITH THE LC-MS 8060RX <i>Jules Griffin, Professor, The Rowett Institute, University of Aberdeen, UK</i> SICRIT® – NEW DIMENSIONS IN MASS SPECTROMETRY <i>Jan Bucek, Head of Global Sales, Plasmion GmbH</i>	Salon C2

1:30 p.m. – 3:00 p.m.	Session 4. Multi-Omics <i>Session Chairs: Nicola Zamboni & Ellen De Paepe</i>	Salon E
1:30 p.m. – 1:50 p.m.	4.1 MEANtools integrates multi-omics data to identify metabolites and predict biosynthetic pathways <i>Kumar Saurabh Singh, Maastricht University, Netherlands</i>	202
1:50 p.m. – 2:05 p.m.	4.2 Integrated Blood Multi-Omics with 3D Probability Modelling Predicts Progression and Neuropathological Trajectory ★ <i>Tereza Kacerova, University of Oxford, United Kingdom</i>	164
2:05 p.m. – 2:25 p.m.	4.3 MetaboExpress: A Network-Based Framework for Discovering Gene–Function Relationships in Plants <i>Gerd U. Balcke, IPB-Halle, Germany</i>	174
2:25 p.m. – 2:40 p.m.	4.4 Annotation-independent construction of disease similarity networks from untargeted multi-cohort breath metabolomics ★ <i>Britta Brugger, University Basel, Switzerland</i>	98
2:40 p.m. – 3:00 p.m.	4.5 Inflammation Reprograms the Liver Lipidome and Metabolome: A Multi Omics Map of LPS Response <i>Francisco Javier Rupérez, Universidad San Pablo CEU, Spain</i>	254

TECHNOLOGY ADVANCEMENTS

PLANTS, FOOD, ENVIRONMENT AND MICROBES

★ AWARD WINNERS

Monday, June 22		
Time	Session	Abstract #
1:30 p.m. – 3:00 p.m.	Session 5. Standardization and Multi-Site Validation <i>Session Chairs: Anne Bendt & David Wishart</i>	Salon C1
1:30 p.m. – 1:50 p.m.	5.1 Mapping the Blood Microsample Metabolome: A Multi-Platform Inter-Laboratory Study ★ <i>Daniel Marques De Sa e Silva, Aristotle University of Thessaloniki, Greece</i>	117
1:50 p.m. – 2:05 p.m.	5.2 PLATINUM SPONSOR Quant-ready untargeted metabolomics through scanning-Q1 DIA: ZT Scan DIA <i>Paul Baker, SCIEX, United States</i> 	486
2:05 p.m. – 2:25 p.m.	5.3 Hospital-derived pooled plasma reference material for clinical metabolomics ★ <i>Barbora Pisklakova, Oslo University Hospital, Norway</i>	94
2:25 p.m. – 2:40 p.m.	5.4 GOLD SPONSOR Advancing High-Resolution LC-MS Methods for High Sensitivity Metabolomics <i>David Heywood, Waters Corporation, United Kingdom</i> 	483
2:40 p.m. – 3:00 p.m.	5.5 Preservation of Biological Variation Across Laboratories: A Fed-Fasted Multi-Site Ring Trial <i>Anne Evans, Metabolon, United States</i>	142
1:30 p.m. – 3:00 p.m.	Session 6. Microorganisms <i>Session Chairs: Karl Burgess & Silvia Radenkovic</i>	Salon C2
1:30 p.m. – 1:50 p.m.	6.1 Complex metabolism in a simple system: cell-free metabolomics <i>Mark Styczynski, Georgia Institute Of Technology, United States</i>	280
1:50 p.m. – 2:05 p.m.	6.2 PLATINUM SPONSOR How DIA with mass stability enhances your metabolomics workflow <i>Laudicéia Alves de Oliveira, Shimadzu, Brazil</i> 	488
2:05 p.m. – 2:25 p.m.	6.3 Metabolic plasticity of an Andean lichen mycobiont (<i>Stereocaulon</i> sp.) revealed by untargeted LC-MS and GC-MS metabolomics ★ <i>Christian Matías, Pontificia Universidad Católica del Perú, Peru</i>	233
2:25 p.m. – 2:40 p.m.	6.4 Substrate-Driven Metabolomic Reprogramming and Bioactive Discovery in Lactic Acid Bacteria ★ <i>Golnaz Heidari, Massey University, New Zealand</i>	41
2:40 p.m. – 3:00 p.m.	6.5 Metabolomic evidence of fungal signatures associated with soybean seed rot in Brazil ★ <i>Paula Derksen Macruz, State University of Maringá, Brazil</i>	257

Monday, June 22		
Time	Session	Abstract #
3:30 p.m. – 5:15 p.m.	Session 7. Neurological Disorders <i>Session Chairs: Rima Kaddurah-Daouk & Ambrin Farizah Babu</i>	Salon E
3:30 p.m. – 3:50 p.m.	7.1 Rapid Ambient Metabolomic Profiling of Sebum for Parkinson's Disease Biomarker Discovery Using Paper Spray Ionization-Ion Mobility Mass Spectrometry <i>Breanna Dixon, University Of Manchester, United Kingdom</i>	140
3:50 p.m. – 4:10 p.m.	7.2 Combining spatial metabolomics and transcriptomics to understand long term changes in the brain following a TBI <i>Alex Dickens, University Of Turku, Finland</i>	267
4:10 p.m. – 4:30 p.m.	7.3 Does lipid metabolism play a central role in Late Onset Alzheimer's disease? Evidence from human cohorts and murine models <i>Julian Griffin, University of Aberdeen, United Kingdom</i>	121
4:30 p.m. – 4:50 p.m.	7.4 Unravelling metabolic drivers of neurodegeneration: Cross-species convergence from a Leigh syndrome model <i>Roan Louw, North-West University, South Africa</i>	88
4:50 p.m. – 5:10 p.m.	7.5 UPLC-MS/MS Method to Evaluate a Neurotransmitter Panel in Women Using Cannabis During Pregnancy <i>Corentin Fracapane, Université de Sherbrooke, Canada</i>	169
3:30 p.m. – 5:15 p.m.	Session 8. Analytical Methods and Workflow Innovations <i>Session Chairs: Facundo Fernandez & María Eugenia Monge</i>	Salon C1
3:30 p.m. – 3:50 p.m.	8.1 A Validated Single-Tube Dual-Extraction Platform for Combined Placental Metabolomics and Lipidomics to Investigate In Utero Exposures <i>Ellen De Paepe, Ghent University, Belgium</i>	250
3:50 p.m. – 4:10 p.m.	8.2 A tailored HILIC–TIMS–MS strategy to unlock Bis(monoacylglycero)phosphates profiling in lysosomal disorders <i>Fabrizio Merciai, University of Salerno, Italy</i>	266
4:10 p.m. – 4:30 p.m.	8.3 Helios2D: A Cell-Preserving Method for Mass Spectrometric Analysis of Living Cells under Near-Native Conditions <i>Timm Schaeffle, University of Tübingen, Germany</i>	134
4:30 p.m. – 4:50 p.m.	8.4 Workflow optimization for integrated mass spectrometry-based metabolomics and lipidomics from dried blood microsamples <i>Eleonora Bossi, University Of Milano-bicocca, Italy</i>	35
4:50 p.m. – 5:10 p.m.	8.5 A Multiomics Approach to Understanding and Targeting Glioblastoma <i>Elizabeth Want, Imperial College London, United Kingdom</i>	166

★ AWARD WINNERS

Monday, June 22		
Time	Session	Abstract #
3:30 p.m. – 5:15 p.m.	Session 9. Food <i>Session Chairs: Sastia Putri & Carolina T. S. D'Almeida</i>	Salon C2
3:30 p.m. – 3:50 p.m.	9.1 Value chain-oriented Metabolomics: Integrating agrobiodiversity bioprospecting with process optimization for functional food design-A Green Onion Case Study ★ <i>Mateo Mejia, Universidad EAFIT, Colombia</i>	83
3:50 p.m. – 4:10 p.m.	9.2 Transition Dairy Cow Health: A Multiomics Approach <i>Simone Rochfort, Agriculture Victoria Research, Australia</i>	20
4:10 p.m. – 4:30 p.m.	9.3 Untargeted UHPLC–Ion Mobility–MS Metabolomics for Scottish Honey Authentication: Geographic, Seasonal, and Blend Signatures ★ <i>Renata Garbellini Duft, University of Aberdeen, United Kingdom</i>	167
4:30 p.m. – 4:50 p.m.	9.4 Untargeted Metabolomics Applied to Study the Chemical Composition of Propolis from Vale do Jequitinhonha (Brazil) <i>Adriana Nori De Macedo, Federal University of Minas Gerais, Brazil</i>	262
4:50 p.m. – 5:10 p.m.	9.5 Discovery-driven untargeted metabolomics reveals compound transformations during static in vitro gastrointestinal digestion of cereal matrices <i>Luciana Lima, UNIRIO, Brazil</i>	38

★ **AWARD WINNERS**

Tuesday, June 23		
Time	Session	Abstract #
8:30 a.m. – 9:30 a.m.	Plenary Session 3 <i>Huiru Tang, Fudan University, China</i> Quantitative Metabolomics: Challenges and New Findings	<i>Salon E</i>
10:15 a.m. – 12:00 p.m.	Session 10. Microbiota & Infectious Disease <i>Session Chairs: Rick Dunn & Breanna Dixon</i>	<i>Salon E</i>
10:15 a.m. – 10:45 a.m.	10.1 KEYNOTE Dietary Determinants of Colorectal Cancer Risk: From Association to Causation <i>Jia Li, Imperial College London, United Kingdom</i>	365
10:45 a.m. – 11:05 a.m.	10.2 Imidazole Propionate: From Untargeted Metabolomics Discovery to a Mechanistic Driver of Atherosclerosis <i>Annalaura Mastrangelo, Spanish National Center for Cardiovascular Research, Spain</i>	93
11:05 a.m. – 11:20 a.m.	10.3 Intramammary milk transplantation induces microbial and metabolic remodeling in experimental caprine mastitis ★ <i>Ana Júlia Silva Moreira, Federal University of Vicosa, Brazil</i>	231
11:20 a.m. – 11:40 a.m.	10.4 Integrated Multiplatform Metabolomics and Microbiota Profiling of HPV Infection in an Underdiagnosed Rural Peruvian Cohort <i>Victor González-Ruiz, CEU-San Pablo University, Spain</i>	185
11:40 a.m. – 12:00 p.m.	10.5 Untargeted Metabolomics Reveals HIV and cART-Associated Metabolic Changes Linked to Cardiovascular Risk <i>Jacques-gernore Frans, North-West University, South Africa</i>	306
10:15 a.m. – 12:00 p.m.	Session 11. Machine Learning and AI Systems <i>Session Chairs: Tim Ebbels & Soha Hassoun</i>	<i>Salon C1</i>
10:15 a.m. – 10:45 a.m.	11.1 KEYNOTE From Rigid to Self-Evolving Multi-Agent AI System for Metabolomics <i>Louis-Félix Nothias, CNRS & Université Côte d'Azur, France</i>	363
10:45 a.m. – 11:05 a.m.	11.2 Adduct-Specific Machine Learning for Accurate Collision Cross Section Prediction in Untargeted Metabolomics <i>Facundo Fernandez, Georgia Institute of Technology, United States</i>	195
11:05 a.m. – 11:20 a.m.	11.3 Aligning Metabolomic Networks via Graph Learning for Common Subnetwork Discovery <i>Edwin Alvarez Mamani, Pontificia Universidad Católica del Perú, Peru</i>	232
11:20 a.m. – 11:40 a.m.	11.4 Deriving Insights from Mass Spectrometry Imaging and Single Cell Datasets with Biologically Informed Neural Networks <i>Thomas Rix, Imperial College London, United Kingdom</i>	239
11:40 a.m. – 12:00 p.m.	11.5 Multimodal Mass Spectrometry Imaging Data Integration using Machine Learning and Network Analyses ★ <i>Lukas Kopecky, Imperial College London, United Kingdom</i>	256

★ AWARD WINNERS

Tuesday, June 23		
Time	Session	Abstract #
10:15 a.m. – 12:00 p.m.	Session 12. Ion Mobility and Integrated Workflows <i>Session Chairs: Coral Barbas & Renata Garbellini Duft</i>	Salon C2
10:15 a.m. – 10:45 a.m.	12.1 KEYNOTE The role of chromatography and ion mobility in metabolite identification ★ <i>Michael Witting, Helmholtz Zentrum Muenchen, Germany</i>	375
10:45 a.m. – 11:05 a.m.	12.2 Cyclic Ion Mobility Separations of Oxidized Free Fatty Acids <i>Eric Gier, Georgia Institute of Technology, United States</i>	39
11:05 a.m. – 11:20 a.m.	12.3 PLATINUM SPONSOR Transforming Metabolomics with Breakthrough NMR and MS Technologies <i>Erica Forsberg, Bruker, United States</i>	 484
11:20 a.m. – 11:40 a.m.	12.4 Toward integration of enantiomeric resolution into mass spectrometry-based metabolomics workflows through fragmentation of non-covalent complexes <i>Annelaure Damont, CEA, France</i>	73
11:40 a.m. – 12:00 p.m.	12.5 Uniting targeted quantification and untargeted ion mobility in one unified workflow for small molecule analysis <i>Alice Limonciel, biocrates life sciences ag, Austria</i>	206

Tuesday, June 23		
Time	Session	Abstract #
12:20 p.m. – 1:20 p.m.	Sponsor Lunch Presentations	
 Agilent	Agilent Technologies From Targeted analysis of VOCs to Lipidomics and Data Integration: The CEMBIO Experience with Agilent Platforms in Translational Metabolomics <i>Dr. Coral Barbas Arribas, Professor, Universidad San Pablo CEU</i>	Salon E
 BRUKER	Bruker What's for Dinner? timsMetabo™-based Metabolomics and Lipidomics of Omnivore and Vegetarian Human Fecal Reference Material NIST RM 8048 <i>Dr. Michael Witting, Deputy Head Metabolomics and Proteomics, Core, Helmholtz Munich, Germany</i> Phenomic Medicine: Application of NMR Molecular Data to Enhance Patient Outcomes <i>Prof Julien Wist, Professor of Computational Spectroscopy, Universidad del Valle, Colombia</i>	Salon C1
 ThermoFisher SCIENTIFIC	Thermo Fisher Scientific Debating the Dark Metabolome: Technologies to Illuminate the Unknown Panel Discussion: <i>Rick Dunn, Professor of Analytical and Clinical Metabolomics, University of Liverpool; Yasin El Abied, Postdoctoral Researcher, Institute of Analytical Chemistry, BOKU University; Jennifer Kirwan, Professor of Veterinary Metabolomics, University of Veterinary Medicine Vienna; Nicola Zamboni, Professor and Principal Investigator, Institute of Molecular Systems Biology, ETH Zurich</i>	Salon C2

★ AWARD WINNERS

Tuesday, June 23		
Time	Session	Abstract #
1:30 p.m. – 3:00 p.m.	Session 13. Immunometabolism and Infectious Disease <i>Session Chairs: Aurelia Williams & Yamilé Lopes Hernandez</i>	Salon E
1:30 p.m. – 1:50 p.m.	13.1 Serum NMR Metabolomics Directed Multi-omics Investigation of Acute Respiratory Distress Syndrome (ARDS) Severities and Their System Biology Pathways <i>Leo Cheng, Corewell Health Research Institute, United States</i>	48
1:50 p.m. – 2:05 p.m.	13.2 PLATINUM SPONSOR Connecting Metabolomics to Function: A Unified Platform for Actionable Biology <i>Fernando (Ralph) Tobias, Agilent Technologies, United States</i>	 Agilent 487
2:05 p.m. – 2:25 p.m.	13.3 Unraveling new pathways in sepsis pathogenesis using LC-MS/MS-based metabolic profiling <i>Andrea Gerdemann, University of Muenster, Germany</i>	288
2:25 p.m. – 2:40 p.m.	13.4 Simultaneous quantitative and qualitative analysis of oxylipins using high resolution mass spectrometry with CID and EAD based fragmentation <i>Paul Baker, SCIEX, United States</i>	268
2:40 p.m. – 3:00 p.m.	13.5 COVID Dogolomics: Integrating Canine Olfaction and GC-MS Volatilomics to Identify Urinary VOC Signatures of Post COVID Syndrome ★ <i>Lea Woyciechowski, TU Braunschweig, Germany</i>	283
1:30 p.m. – 3:00 p.m.	Session 14. Real-Time Analysis <i>Session Chairs: Lynn VanHaecke & Shauni Loopmans</i>	Salon C1
1:30 p.m. – 1:50 p.m.	14.1 Integrated real-time breath analysis for therapeutic drug monitoring and outcome prediction in epilepsy <i>Pablo Sinues, University of Basel, Switzerland</i>	201
1:50 p.m. – 2:05 p.m.	14.2 SPONSOR Software, hardware and intelligent acquisition strategies for guided unknown metabolite characterization <i>Susan S. Bird, Thermo Fisher Scientific, United States</i>	 ThermoFisher SCIENTIFIC 485
2:05 p.m. – 2:25 p.m.	14.3 Real-time metabolomic approach for the monitoring of Chinese hamster ovary cell metabolism <i>Yuandi Zhao, University of Edinburgh, United Kingdom</i>	92
2:25 p.m. – 2:40 p.m.	14.4 Urinary Metabolome dynamics in 13C-labeled mice <i>Eric Ezan, CEA, France</i>	28
2:40 p.m. – 3:00 p.m.	14.5 Real Time Metabolomics and Bayesian Optimization for Surfactant Production in Bacillus subtilis ★ <i>Catalina Guerra, University of Edinburgh, United Kingdom</i>	118

★ AWARD WINNERS

Tuesday, June 23		
Time	Session	Abstract #
1:30 p.m. – 3:00 p.m.	Session 15. Plants and Food <i>Session Chairs: Ian Castro-Gamboa & Art Edison</i>	Salon C2
1:30 p.m. – 1:50 p.m.	15.1 Integrated metabolomics reveals genotype-driven phenolic diversity in sorghum germplasm <i>Carolina T. S. D'Almeida, Federal University of the State of Rio de Janeiro, Brasil</i>	104
1:50 p.m. – 2:05 p.m.	15.2 Anaerobic processing enhances γ -aminobutyric acid (GABA) production and α -glucosidase inhibitory activity in tempe <i>Chiaki Tsushi, Shimadzu Corporation, Japan</i>	109
2:05 p.m. – 2:25 p.m.	15.3 The MetaBó-Bainne Study – Characterisation of the milk metabolome from a seasonal pasture-based dairy system using ^1H -NMR spectroscopy ★ <i>Paula Rojas Gómez, University College Cork, Ireland</i>	90
2:25 p.m. – 2:40 p.m.	15.4 Untargeted Metabolomics Integration of MS and NMR for the Taxonomic Investigation of Psychotria and Palicourea <i>Daniele De Oliveira Silva, Federal University of Alfenas, Brazil</i>	150
2:40 p.m. – 3:00 p.m.	15.5 Untargeted UHPLC-HD-QTOF/MS Metabolomics Reveals Pathway-Level Modes of Action and Defence Priming by Laminarin and Paenibacillus alvei T22 in Triticum aestivum ★ <i>Manamele Dannies Mashabela, University Of Johannesburg, South Africa</i>	177
3:30 p.m. – 5:15 p.m.	Session 16. Chemical Exposures and Bioactive Metabolites <i>Session Chairs: Du Toit Loots & Elizabeth Want</i>	Salon E
3:30 p.m. – 3:50 p.m.	16.1 Plasma-Based Biomonitoring of Environmental PAH Exposure Using a Targeted GC-MS/MS Exposomics Platform <i>Jutarop Phetcharaburanin, Khon Kaen University, Thailand</i>	261
3:50 p.m. – 4:10 p.m.	16.2 Integrating the chemical exposome into metabolomics via the ExpoLib spectral library and newborn screening programs <i>Vinicius Verri Hernandez, University of Vienna, Austria</i>	215
4:10 p.m. – 4:30 p.m.	16.3 High-throughput Urine Exposomic Studies for Global Health: Deciphering Cigarette Smoke and Coffee Co-exposures...A Bad Combination? <i>Philip Britz-McKibbin, McMaster University, Canada</i>	265
4:30 p.m. – 4:50 p.m.	16.4 Untargeted Metabolomics and Type 2 Diabetes Incidence: A Prospective Multi-cohort study in European Populations <i>Robert van Vorstenbosch, Institute for Risk Assessment Sciences, Utrecht University, Netherlands</i>	136
4:50 p.m. – 5:10 p.m.	16.5 LC-HRMS Metabolomics of Plasma Samples: Diagnosing Interferences, Contaminants and Matrix Effects Using Post-Column Infusion of Stable Isotope-Labelled Standards <i>Daniel Malheiro, University of Copenhagen / Cmbio, Denmark</i>	23

★ **AWARD WINNERS**

Tuesday, June 23		
Time	Session	Abstract #
3:30 p.m. – 5:15 p.m.	Session 17. Data Ecosystems and Knowledge Sharing <i>Session Chairs: Roy Goodacre & Thomas Dussarrat</i>	Salon C1
3:30 p.m. – 3:50 p.m.	17.1 MetabolomicsHub: International Data Exchange and Data Representation Standards for Metabolomics <i>Callum Martin, EMBL-EBI, United Kingdom</i>	190
3:50 p.m. – 4:10 p.m.	17.2 FASSTrecords and StructureMASST: Unifying Public Metabolomics Data for Worldwide Metabolome Exploration ★ <i>Yasin El Abiead, BOKU University, Austria</i>	251
4:10 p.m. – 4:30 p.m.	17.3 Mass Spectral Library Network (MERLIN) To Streamline The Generation Of Public Spectral Libraries. <i>Federico Brigante, Institute Of Organic Chemistry And Biochemistry, Czech Republic</i>	63
4:30 p.m. – 4:50 p.m.	17.4 Beyond altruism: How open research maximizes your scientific impact. <i>Philippine Louail, Institute for Biomedicine, Eurac Research, Italy</i>	91
4:50 p.m. – 5:10 p.m.	17.5 OmniPath Metabo: database and tools for mechanistic modeling and analysis of metabolomics data <i>Christina Schmidt, University Clinics Heidelberg, Germany</i>	51
3:30 p.m. – 5:15 p.m.	Session 18. Environment I <i>Session Chairs: Tuulia Hyötyläinen & Alan Pilon</i>	Salon C2
3:30 p.m. – 3:50 p.m.	18.1 Heat, Halogens, and Holobionts: Seasonal Metabolomic and Microbiome Dynamics in the Invasive Red Alga <i>Asparagopsis taxiformis</i> <i>Tal Luzzatto Knaan, University of Haifa, Israel</i>	96
3:50 p.m. – 4:10 p.m.	18.2 Biodiversity effects on oak leaf litter volatilome and implications for soil macrofauna ★ <i>Gabriela A. S. Escalante, German Centre for Integrative Biodiversity Research (iDiv), Germany</i>	222
4:10 p.m. – 4:30 p.m.	18.3 Environmental Metabolic Footprinting (EMF): A New Framework for Assessing the Fate and Impact of Complex Biocontrol Natural Extracts in Soil <i>Cedric Bertrand, Universite De Perpignan, France</i>	204
4:30 p.m. – 4:50 p.m.	18.4 Integrated NMR-MS Metabolomics Reveals Climate-Dependent Neuroprotective Signatures in Mangrove Species <i>Jordan Kahfi, King Abdullah University of Science and Technology, Saudi Arabia</i>	130
4:50 p.m. – 5:10 p.m.	18.5 Compound-class-based profiling for comprehensive untargeted metabolome analysis <i>Pilleriin Peets, University of Tartu, Estonia</i>	21

★ AWARD WINNERS

Wednesday, June 24		
Time	Session	Abstract #
9:30 a.m. – 10:30 a.m.	Plenary Session 4 <i>Fidele Tugizimana, University of Johannesburg, South Africa</i> From African Biodiversity to Global Innovation: AI-Enabled Metabolomics for Plants, Natural Products, and Sustainable Futures	Salon E
11:30 a.m. – 1:15 p.m.	Session 19. Environment II <i>Session Chairs: Matej Orešič & Marina Amaral</i>	Salon E
11:30 a.m. – 12:00 p.m.	19.1 SESSION KEYNOTE Development and validation of a fecal steroidomics workflow for wildlife endocrine monitoring <i>Tom Cools, Leibniz Institute for Zoo and Wildlife Research, Germany</i>	176
12:00 p.m. – 12:20 p.m.	19.2 Selective sequestration and differential tissue distribution of xenobiotics in the poison frog <i>Phylllobates terribilis</i> : A quantitative HPLC-MS/MS study ★ <i>Mabel Gonzalez, Stanford University, United States</i>	295
12:20 p.m. – 12:35 p.m.	19.3 Untargeted DI-HRMS Metabolomics Reveals UV-A-Induced Metabolic Plasticity in High-Andean Lichen Species ★ <i>Erika Lizet Milagros Calla Quispe, Pontificia Universidad Católica del Perú, Peru</i>	234
12:35 p.m. – 12:55 p.m.	19.4 PFAS Exposure Modulates Mitochondrial Susceptibility in Steatotic Hepatocytes ★ <i>João Marcos Barbosa, Örebro University, Sweden</i>	132
12:55 p.m. – 1:15 p.m.	19.5 Seasonal Metabolite Profiling of <i>Thyone aurea</i> from Saldanha Bay, South Africa ★ <i>Cassandra Upton, University of South Africa, South Africa</i>	184
11:30 a.m. – 1:15 p.m.	Session 20. Cancer Metabolomics <i>Session Chairs: Roan Louw & Cristina Andres-Lacueva</i>	Salon C1
11:30 a.m. – 12:00 p.m.	20.1 KEYNOTE Uncovering the Heterogeneity of the Human Metabolome <i>Rafael Montenegro Burke, University Of Toronto, Canada</i>	364
12:00 p.m. – 12:20 p.m.	20.2 Metabolomic Landscape of IPMN cyst fluid reveals signatures of pancreatic cancer progression <i>Eduardo Sommella, University of Salerno, Italy</i>	241
12:20 p.m. – 12:35 p.m.	20.3 Metabolomic signatures of low-insulinemic and anti-inflammatory dietary patterns in relation to colorectal cancer risk across global populations <i>Fred Tabung, Ohio State University, United States</i>	126
12:35 p.m. – 12:55 p.m.	20.4 Metabolomic and proteomic profiling in an underrepresented population reveals novel molecular risk factors for gastric cancer <i>Xiang Shu, Memorial Sloan Kettering Cancer Center, United States</i>	200
12:55 p.m. – 1:15 p.m.	20.5 Targeting the K-RAS4B/PDE6 _γ Complex Reveals Differential Lipid Metabolic Responses in Pancreatic Cancer Cells ★ <i>Sandra Delfín-Azuara, CINVESTAV, Mexico</i>	199

★ AWARD WINNERS

Wednesday, June 24		
Time	Session	Abstract #
11:30 a.m. – 1:15 p.m.	Session 21. Nutrimetabolomics <i>Session Chairs: Mónica Cala & Juan José Oropeza Valdez</i>	Salon C2
11:30 a.m. – 12:00 p.m.	21.1 KEYNOTE Decoding Variability in Dietary Response: A Metabolic Phenotyping Approach for Personalised Nutrition <i>Isabel Garcia Perez, Imperial College Healthcare NHS Trust, United Kingdom</i>	373
12:00 p.m. – 12:20 p.m.	21.2 An Integrated Untargeted and Targeted LC-MS Metabolomics Approach to Characterise the Systemic Effects of S-Methyl Cysteine Sulfoxide in Diet-Induced Metabolic Syndrome <i>Armaghan Shafaei, Edith Cowan University, Australia</i>	50
12:20 p.m. – 12:35 p.m.	21.3 High throughput ex vivo stable isotope tracing using tissue homogenates to model in vivo metabolism <i>Shauni Loopmans, KU Leuven – VIB, Belgium</i>	305
12:35 p.m. – 12:55 p.m.	21.4 Nontargeted metabolomics reveals changes in plasma metabolome after an oat-rich low-gluten diet with candidate biomarkers of oat consumption ★ <i>Enni Mannila, University of Turku, Finland</i>	25
12:55 p.m. – 1:15 p.m.	21.5 Lipidomic Fingerprinting Reveals Bioactive Signatures of Human Milk Extracellular Vesicles <i>Julia Kuligowski, Health Research Inst. La Fe, Spain</i>	87
1:35 pm – 2:35 pm	Town Hall Meeting <i>Rick Dunn, President, Metabolomics Society</i>	Salon E
2:45 p.m. – 4:30 p.m.	Plenary Session 5 Awards & Closing <i>Mariana Simões Larraz Ferreira, Federal University of the State of Rio de Janeiro (UNIRIO), Brazil</i> Metabolomics-driven cereal biotechnology: phenolic diversity, gastrointestinal transformation, and geographical indication	Salon E