METABOLOMICS
SOCIETY

20th Annual Conference of the Metabolomics Society

METABOLOMICS2024

OSAKA, JAPAN

JUNE 16-20

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 16

	Hall C	Hall D	Hall E
11:00 a.m.	**REGISTRATION OPEN**		
12:00 p.m. – 2:00 p.m.	**W1:** Nutritional Metabolomics: Biomarkers of Dietary Intake and Exposure	**W2:** Public Data Re-use / Re-analysis w/ MetaboLights and GNPS	**W3:** Untargeted Met, Molecular Networking, Mzmine
2:00 p.m. – 2:15 p.m.	**BREAK**		
2:15 p.m. – 4:15 p.m.	**W4:** Demystifying Stable Isotope Labelling	**W5:** SIRIUS 6 for Small Molecule Annotation Using MS/MS Data	**W6:** Part 1 MetaboAnalyst 6.0
4:30 p.m. – 6:30 p.m.		**W7:** Reconnecting Lipidomics and Metabolomics for Metabolic Research	**W6:** Part 2 MetaboAnalyst 6.0
6:45 p.m. – 8:00 p.m.	**Career Night – Roundtable Discussions | Hall C**		

MONDAY, JUNE 17

	Hall C	Hall D	Hall E
7:30 a.m.	**REGISTRATION / INFO DESK OPEN**		
8:15 a.m. – 10:15 a.m.	**W8:** Unveiling the mQACC Living Guidance for QA/QC Best Practices	**W9:** EMN Professional Career Development	**W10:** Improving Data Analysis for Ambient Ionisation
10:15 a.m. – 10:30 a.m.	**BREAK**		
10:30 a.m. – 12:30 p.m.	**W11:** Metabolomics Infrastructure and Facility Forum	**W12:** FAIR and Open Data Sharing through Public Repositories	**W13:** MALDI-MS Imaging Tool for Medical Prognosis
12:30 p.m. – 1:30 p.m.	**LUNCH BREAK *(on your own)***		
1:30 p.m. – 3:00 p.m.	**Opening Ceremony & Plenary Session 1** – Pieter Dorrestein | Hall A		
3:00 p.m. – 3:30 p.m.	**BREAK**		
	Hall A	**Hall D**	**Hall E**
3:30 p.m. – 5:10 p.m.	🟦 **1** Microbiome Applications	🟨 **2** Metabolite Annotation	🟧 **3** Toward Single Cell Analysis
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 | Hall A**		

TUESDAY, JUNE 18

	Hall A	Hall D	Hall E
8:00 a.m.	**REGISTRATION / INFO DESK OPEN**		
8:30 a.m. – 9:30 a.m.	**Plenary Session 2 –** Jules Griffin | Hall A		
9:30 a.m. – 10:15 a.m.	**BREAK**		
10:15 a.m.– 12:00 p.m.	🟧 **4** Analytical Quality Management	🟨 **5** Mining Data Repositories	🟩 **6** Environmental Exposures
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:** Thermo Fisher Scientific
1:30 p.m. – 3:00 p.m.	🟦 **7** NutriMet & Dietary Biomarkers	🟨 **8** Multiomics and Data Integration	🟧 **9** Technology Advancements
3:00 p.m. – 3:30 p.m.	**BREAK**		
3:30 p.m. – 5:10 p.m.	**10** Vendor Session	🟦 **11** Met and Lipidomics in Cardiovascular Research	🟩 **12** Microbial Metabolomics
5:15 p.m. – 6:45 p.m.	**Poster Session 2**		
7:00 p.m. – 8:30 p.m.	**EMN Reception | Hall C**		

WEDNESDAY, JUNE 19

	Hall A	Hall D	Hall E
8:00 a.m.	**REGISTRATION / INFO DESK OPEN**		
8:30 a.m. – 9:30 a.m.	**Plenary Session 3** – Kazuki Saito | Hall A		
9:30 a.m. – 10:15 a.m.	**BREAK**		
10:15 a.m. – 12:00 p.m.	🟦 **13** Metabolic Health	🟨 **14** Machine Learning of Metabolics Data	🟩 **15** Marine and Freshwater Metabolomics
12:00 p.m. – 1:30 p.m.	**LUNCH BREAK AND SPONSOR PRESENTATIONS**		
12:20 p.m. – 1:20 p.m.		**Sponsor Pres:** AB SCIEX	**Sponsor Pres:** Bruker
1:30 p.m. – 3:00 p.m.	🟦 **16** Neurological Diseases	🟩 **17** Food Metabolomics	🟦 **18** Liver Diseases
3:00 p.m. – 3:30 p.m.	**BREAK**		
3:30 p.m. – 5:10 p.m.	🟦 **19** Maternal and Neonatal Health	🟨 **20** Data Processing and Statistics	🟧 **21** Imaging and Fluxomics
5:15 p.m. – 6:45 p.m.	**Poster Session 3**		
7:30 p.m. – 11:00 p.m.	**Conference Dinner**		

THURSDAY, JUNE 20

	Hall A	Hall D	Hall E
8:15 a.m.	**REGISTRATION / INFO DESK OPEN**		
8:30 a.m. – 9:30 a.m.	**Plenary Session 4** – Claudia Langenberg | Hall A		
9:30 a.m. – 10:30 a.m.	**Poster Session 4**		
10:30 a.m. – 12:10 p.m.	🟦 **22** Cancer	🟩 **23** Plant Metabolomics	🟧 **24** Non-targeted and Semi-targeted Methods
12:15 p.m. – 1:30 p.m.	**LUNCH BREAK AND SPONSOR PRESENTATIONS**		
12:25 p.m. – 1:25 p.m.		**Sponsor Pres:** Shimadzu Corporation	**Sponsor Pres:** Waters Corporation
1:30 p.m. – 3:15 p.m.	**Plenary Session 5** – Yu Xia – **Awards and Closing** | Hall A		

🟦 **METABOLOMICS IN HEALTH AND DISEASE**
🟨 **COMPUTATIONAL METABOLOMICS, STATISTICS & BIOINFORMATICS**

★ **AWARD WINNERS**

Monday, June 17

Time	Session	Abstract #
1:30 p.m. – 3:00 p.m.	**Opening Ceremony & Plenary Session 1** *Pieter Dorrestein, University of California San Diego, United States* The Emergence of the Big Data Era in Metabolomics – Discovering New Biology Across Metabolomics Repositories	***Hall A***
3:30 p.m. – 5:10 p.m.	**Session 1. Microbiome Applications** *Session Chairs: Lynn Vanhaecke and Silvia Radenkovic*	***Hall A***
3:30 p.m. – 4:00 p.m.	**1.1 KEYNOTE** Studies on gut microbial dietary and medicinal component metabolisms and its application to metabolomics and health promotion *Jun Ogawa, Kyoto University, Japan*	**458**
4:00 p.m. – 4:20 p.m.	**1.2** Microbiome derived bile acids during early life: Insights into the progression to islet autoimmunity *Matej Orešič, Örebro University, Sweden*	**290**
4:20 p.m. – 4:35 p.m.	**1.3** Advanced metabolomics for the investigation of gut microbiota-derived metabolites using chemical biology tools *Ioanna Tsiara, Uppsala University, Sweden*	**166**
4:35 p.m. – 4:55 p.m.	**1.4** Inhibition of IRAK4 by microbial trimethylamine blunts metabolic inflammation and ameliorates glycemic control *Marc-Emmanuel Dumas, CNRS and Imperial College London, France*	**407**
4:55 p.m. – 5:10 p.m.	**1.5** Oral microbiome associates with salivary metabolome and sugars profile ★ *Stefania Noerman, Chalmers Univ. of Technology, Sweden*	**270**
3:30 p.m. – 5:10 p.m.	**Session 2. Metabolite Annotation** *Session Chairs: Tim Ebbels and Clary Clish*	***Hall D***
3:30 p.m. – 4:00 p.m.	**2.1 KEYNOTE** Turning tandem mass spectra into metabolite structure information: What is new in SIRIUS 6? *Sebastian Böcker, Friedrich Schiller University Jena, Germany*	**450**
4:00 p.m. – 4:20 p.m.	**2.2** Molecular Networking-Based Global Metabolome Annotation and Key Pathway Exploration *Xin Lu, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China*	**268**
4:20 p.m. – 4:35 p.m.	**2.3** Fiora: Accurate prediction of compound mass spectra from single fragmentation events *Yannek Nowatzky, Bundesanstalt für Materialforschung und Prüfung, Germany*	**153**
4:35 p.m. – 4:55 p.m.	**2.4** Naming Harmonization: the Metabolites Merging Strategy (MMS) for Enhanced Interstudy Comparability *Hector Villalba, Universitat Rovira I Virgili, Spain*	**388**
4:55 p.m. – 5:10 p.m.	**2.5** Untargeted stable isotope labelling studies in lipidomics and metabolomics: two tailored solutions for computer-aided analysis *Laura Goracci, University Of Perugia, Italy*	**175**

★ **AWARD WINNERS**

Monday, June 17

Time	Session	Abstract #
3:30 p.m. – 5:10 p.m.	**Session 3. Toward Single Cell Analysis** *Session Chairs: Takeshi Bamba and Domenica Berardi*	*Hall E*
3:30 p.m. – 4:00 p.m.	**3.1 KEYNOTE** Intact living-cell electrolaunching ionization mass spectrometry for single-cell metabolomics and its application *Xiayan Wang, Beijing University Of Technology, China*	**433**
4:00 p.m. – 4:20 p.m.	**3.2** Untargeted single cell lipidomics using trapped ion mobility spectrometry *Erica Forsberg, Bruker Daltonics, United States*	**220**
4:20 p.m. – 4:35 p.m.	**3.3** Large-Scale and In-Depth Single-Cell Metabolomics Enabled by Ion Mobility-Mass Spectrometry *Mingdu Luo, Chinese Academy of Sciences, China*	**73**
4:35 p.m. – 4:55 p.m.	**3.4** Cell cycle-dependent single-cell multi-omics analysis *Yoshihiro Izumi, Kyushu University, Japan*	**350**
4:55 p.m. – 5:10 p.m.	**3.5** Unlocking the Potential of Capillary Flow Ion-Exchange Chromatography coupled to Mass Spectrometry for Highly Polar and Ionic Metabolite Analysis ★ *Rachel Williams, University of Oxford, United Kingdom*	**346**

🟧 TECHNOLOGY ADVANCEMENTS
🟨 COMPUTATIONAL METABOLOMICS, STATISTICS & BIOINFORMATICS

Tuesday, June 18

Time	Session	Abstract #
8:30 a.m. – 9:30 a.m.	**Plenary Session 2** *Jules Griffin, University of Aberdeen, United Kingdom* Lipidomics at the population scale to understand the metabolic syndrome – from 50 um to 15000 people	*Hall A*
10:15 a.m. – 12:00 p.m.	**Session 4. Analytical Quality Management** *Session Chairs: Roy Goodacre and Xiayan Wang*	*Hall A*
10:15 a.m. – 10:45 a.m.	**4.1 SESSION KEYNOTE** Effects of adduct formation and internal standard selection on data harmonization in untargeted LC-MS lipidomics *Dajana Vuckovic, Concordia University, Canada*	**390**
10:45 a.m. – 11:05 a.m.	**4.2** Matrix effects matter: a comparative evaluation of urine normalisation methods *Stacey Reinke, Edith Cowan University, Australia*	**136**
11:05 a.m. – 11:20 a.m.	**4.3** Development and Validation of a Multiplex LC-ESI-MS/MS Method for Quantification of Carboxylic Acids in Urine *Guan-yuan Chen, National Taiwan University, Taiwan*	**141**
11:20 a.m. – 11:40 a.m.	**4.4** Comprehensive coverage of glycolysis and pentose phosphate metabolic pathways by isomer-selective targeted hydrophilic interaction liquid chromatography-tandem mass spectrometry assay *Kristian Serafimov, University Of Tübingen, Germany*	**176**
11:40 a.m. – 12 p.m.	**4.5** Breaking the taboo of metabolomics with transparency *Elliott James Price, RECETOX, Masaryk University, Czech Republic*	**239**
10:15 a.m. – 12:00 p.m.	**Session 5. Mining Data Repositories** *Session Chairs: Fabien Jourdan and Masanori Arita*	*Hall D*
10:15 a.m. – 10:45 a.m.	**5.1 KEYNOTE** Making Metabolomics Data FAIR and Sustainable *Masanori Arita, National Institute Of Genetics, Japan*	**464**
10:45 a.m. – 11:05 a.m.	**5.2** Mapping the Evolutionary Chemistry of Life through Public Metabolomics Data Exploration. *Yasin El Abiead, University of California San Diego, United States*	**401**
11:05 a.m. – 11:20 a.m.	**5.3** Reanalysis of public domain, untargeted metabolomics datasets using AI-powered workflow: Unraveling novel biomarkers for severe COVID *Pramod Wangikar, Indian Institute Of Technology Bombay, India*	**207**
11:20 a.m. – 11:40 a.m.	**5.4** The HuMet Repository: An interactive resource of time-resolved metabolite profiles for exploring human metabolism under challenges *Gabi Kastenmüller, Helmholtz Zentrum München, Germany*	**417**
11:40 a.m. – 12 p.m.	**5.5** Deep mining for exposome signatures across multiple data types *Zhiqiang Pang, McGill University, Canada*	**385**

PLANTS, FOOD, ENVIRONMENT AND MICROBES

★ **AWARD WINNERS**

Tuesday, June 18

Time	Session	Abstract #
10:15 a.m. – 12:00 p.m.	**Session 6. Environmental Exposures** *Session Chairs: Michael Witting and David Beale*	*Hall E*
10:15 a.m. – 10:45 a.m.	**6.1 KEYNOTE** Environmental Cheminformatics and Metabolomics – Two Worlds Collide? *Emma Schymanski, LCSB, University Of Luxembourg, Luxembourg*	**449**
10:45 a.m. – 11:05 a.m.	**6.2** Metabolomics and lipidomics to assess neurotoxicity and demyelination in human 3D brain spheres: exposure to cuprizone and bisphenol A *Isabel Meister, University of Geneva, Switzerland*	**400**
11:05 a.m. – 11:20 a.m.	**6.3** Petroleum Derivatives Unseen Influence: Changes in Skin Bacteria and Metabolites ★ *Alan Hernandez, CICESE, Mexico*	**203**
11:20 a.m. – 11:40 a.m.	**6.4** What are the metabolic effects of per-and polyfluoroalkyl substances at environmentally relevant exposures? *Oliver Jones, RMIT University, Australia*	**288**
11:40 a.m. – 12 p.m.	**6.5** Introducing an online-SPE-LC-MS/MS method to examine thyroid hormone concentrations in rat plasma and brain *Jenny Fischer, BASF Metabolome Solutions GmbH, Germany*	**111**
12:20 p.m. – 1:20 p.m.	**Sponsor Lunch Presentations**	
Agilent	**Agilent Technologies** Development of CE-MS Metabolomics and its Application in Cancer *Tomoyoshi Soga, Professor, Keio University*	*Hall D*
ThermoFisher SCIENTIFIC	**Thermo Fisher Scientific** Bridging Discovery and Validation: Advancing Mass Spectrometry for Accelerated Translational Metabolomics *Kevin Cho, Scientist / Director of Operation, Center for Mass Spectrometry and Metabolic Tracing, Department of Chemistry, Department of Medicine* *Bashar Amer, Vertical Marketing Manager - Metabolomics Applications, Thermo Fisher Scientific*	*Hall E*

★ **AWARD WINNERS**

Tuesday, June 18

Time	Session	Abstract #
1:30 p.m. – 3:00 p.m.	**Session 7. Nutrimetabolomics & Dietary Biomarkers** *Session Chairs: Lorraine Brennan and Kati Hanhineva*	***Hall A***
1:30 p.m. – 1:50 p.m.	**7.1** Biomarkers of healthy eating patterns in a multi-ethnic Asian population *Dorrain Low, Nanyang Technological University, Singapore*	**43**
1:50 p.m. – 2:05 p.m.	**7.2** Unlocking Biomarkers as Dietary Assessment Tools in Nutrition Research ★ *Catalina Cuparencu, University Of Copenhagen, Denmark*	**189**
2:05 p.m. – 2:25 p.m.	**7.3** Serum metabolomics for assessing treatment response differences to a single large bolus dose of cholecalciferol in vitamin D deficient critically ill children *Philip Britz-McKibbin, McMaster University, Canada*	**245**
2:25 p.m. – 2:40 p.m.	**7.4** Associations between the fecal and plasma metabolites are characterized by inter-individual variation and modulated by fiber supplementation *Hany Ahmed, University Of Turku, Finland*	**366**
2:40 p.m. – 3:00 p.m.	**7.5** Probiotic influence on gut metabolome in children at risk for celiac disease ★ *Anna Mascellani Bergo, Czech University Of Life Sciences Prague, Czech Republic*	**354**
1:30 p.m. – 3:00 p.m.	**Session 8. Multiomics and Data Integration** *Session Chairs: Claudia Langenberg and Matej Orešič*	***Hall D***
1:30 p.m. – 1:50 p.m.	**8.1** Sherlocking with Multi-omics and a Dash of Molecular Networking Magic to Unravel Secondary Metabolites in Fungi ★ *Isabella Burger, TU Wien, Austria*	**221**
1:50 p.m. – 2:05 p.m.	**8.2** Metabolite-specific inter-individual variability: A meta-analysis of metabolomics datasets and the need for log transformation *Deepti Sahasrabuddhe, Indian Institute Of Technology Bombay, India*	**209**
2:05 p.m. – 2:25 p.m.	**8.3** Spatial multi-omics characterization of epithelial glands reveals novel prognostic signatures in prostate cancer *Abhibhav Sharma, Norwegian University of Science & Tech, Norway*	**126**
2:25 p.m. – 2:40 p.m.	**8.4** Multiomics profiles for early detection of breast cancer within the UK Biobank *Lisa van den Driest, University of Strathclyde, United Kingdom*	**86**
2:40 p.m. – 3:00 p.m.	**8.5** LEOPARD: Missing view completion for multi-timepoint omics data via representation disentanglement and temporal knowledge transfer *Siyu Han, Technical University of Munich, Germany*	**253**

★ AWARD WINNERS

Tuesday, June 18

Time	Session	Abstract #
1:30 p.m. – 3:00 p.m.	**Session 9. Technology Advancements** *Session Chairs: Farhana Pinu and Toshinari Ishii*	***Hall E***
1:30 p.m. – 1:55 p.m.	**9.1** Rapid and self-administrable capillary blood sampling is functionally equivalent to standard venous collections for NMR-based lipoprotein analysis ★ *Jayden Roberts, Australian National Phenome Centre, Australia*	**348**
1:55 p.m. – 2:15 p.m.	**9.2** Automated sequential derivatization for GC-MS based metabolite profiling of human blood *Akrem Jbebli, RECETOX, Czech Republic*	**238**
2:15 p.m. – 2:40 p.m.	**9.3** Developing a Drop-based Microfluidic Method for Mitochondria Sorting and Metabolome Analysis in Arabidopsis thaliana *Claire-line Marais, Bordeaux Metabolome, MetaboHub, INRAE, France*	**360**
2:40 p.m. – 3:00 p.m.	**9.4** Conversion and integration of OMICS data from a prototype, benchtop multi-reflecting time-of-flight (MRT) platform with third-party informatic workflows *Jayne Kirk, Waters Corp, United Kingdom*	**364**

VENDOR SESSION

Tuesday, June 18

Time	Session	Room
3:30 p.m. – 5:15 p.m.	**Session 10. Vendor Session** **(Presented by Platinum and Gold sponsors)** *Session Chairs: Fidele Tugizimana and Kazuki Saito*	*Hall A*
	PLATINUM PRESENTERS: 3:30 p.m. – 4:35 p.m.	
	Thermo Fisher Scientific Bashar Amer, Vertical Marketing Manager, United States **Exploring New Horizons: Innovative Strategies in Metabolomics and Lipidomics Methodologies**	
	Agilent Technologies Daniel Cuthbertson, Director, Global Life Science Research Market, United States **Synergistic Workflow Solutions to Accelerate Metabolomics Research**	
	SCIEX Dr. Rebekah Sayers, Manager Global Strategic Marketing – Small Molecule Omics, UK **Benefits of the ZenoTOF 7600 System for Precise Quantitation and Structural Characterisation of Metabolites**	
	Bruker Claire Cannet, Market Manager Clinical, Germany **Innovative Solutions in Bruker NMR and MS Technologies for Metabolomics and Lipidomics Research**	
	Shimadzu Corporation Yutaka Umakoshi, Application Chemist, Japan **Introduction of Widely Targeted Metabolomics Workflow**	
	Waters Corporation Jayne Kirk, Ph.D, Principal Consulting Product Manager, UK **Pushing the Boundaries of Science with Multi Reflecting Time of Flight Technology**	
	GOLD PRESENTERS: 4:35 p.m. – 5:15 p.m.	
	Owlstone Medical Matteo Tardelli, Senior Biomarker Scientist, UK **Breath Biopsy and the VOC Atlas: An Introduction**	
	Cambridge Isotope Laboratories Dr. Andrew Percy, Senior Applications Scientist, United States **Stable Isotope-Labeled Tools for QC and Quantitation MS Metabolomics**	
	LECO Corporation David Alonso, Application Chemist, United States **Enhancing Semi-Target Metabolomics using Advanced GC-MS Technology & Software Workflow Solutions**	
	Miltenyi Biotec Fumiaki Ogawa, Marketing CA Sorting Product Manager, Japan **Obtain Reliable Data Sets from Cells with Preserved Physiological Function**	

🟦 METABOLOMICS IN HEALTH AND DISEASE
🟩 PLANTS, FOOD, ENVIRONMENT AND MICROBES

★ **AWARD WINNERS**

Tuesday, June 18

Time	Session	Abstract #
3:30 p.m. – 5:10 p.m.	**Session 11. Metabolomics and Lipidomics in Cardiovascular Research** *Session Chairs: Cristina Legido Quigley and Philip Britz-McKibbin*	*Hall D*
3:30 p.m. – 3:50 p.m.	**11.1** Long-chain polyunsaturated fatty acid-containing phosphatidylcholines predict survival rate in patients after heart failure ★ *Aleš Kvasnička, Palacký University Olomouc, Czech Republic*	**261**
3:50 p.m. – 4:10 p.m.	**11.2** Identification of Biomarkers for Risk Stratification of Vascular Conditions in the Hospital Emergency Department *Jing Kai Chang, National University of Singapore, Singapore*	**37**
4:10 p.m. – 4:30 p.m.	**11.3** Application of a Combined Lipidomic and Polygenic Risk Score for Enhanced Risk Stratification of Cardiovascular Disease in Primary Prevention *Jingqin Wu, Baker Heart And Diabetes Institute, Melbourne, Australia*	**156**
4:30 p.m. – 4:50 p.m.	**11.4** Interspecies metabolomic comparison revealed that purine metabolism regulates postnatal cardiomyocyte cell cycle arrest ★ *Yuichi Saito, Laboratory for Heart Regeneration, RIKEN BDR, Japan*	**88**
4:50 p.m. – 5:10 p.m.	**11.5** Prediction of statin usage in large population cohorts using lipidomics data ★ *Changyu Yi, Baker Heart and Diabetes Institute, Australia*	**195**
3:30 p.m. – 5:10 p.m.	**Session 12. Microbial Metabolomics** *Session Chairs: Tomáš Pluskal and Sastia Prama Putri*	*Hall E*
3:30 p.m. – 3:50 p.m.	**12.1** Untargeted metabolic profiling of Mycobacterium tuberculosis identifies a new stress response metabolite *Robert Jansen, Radboud University, Netherlands*	**306**
3:50 p.m. – 4:10 p.m.	**12.2** Exploring Metabolic Vulnerabilities in Antibiotic-Resistant Bacteria Using Untargeted Metabolomics. *Kyoungeun Lee, University Of Oxford, United Kingdom*	**185**
4:10 p.m. – 4:30 p.m.	**12.3** Wielding untargeted metabolomics to explore marine bacteria community interactions ★ *Monica Monge Loria, Georgia Institute of Technology, United States*	**51**
4:30 p.m. – 4:50 p.m.	**12.4** Towards the development of rapid diagnostics for the detection of carbapenem-resistant Enterobacteriaceae *Breanna Dixon, University Of Manchester, United Kingdom*	**61**
4:50 p.m. – 5:10 p.m.	**12.5** Role of Siderophores in Inhibiting the Specialized Metabolism in Fungal-Bacterial Interactions *Huong T. Pham, Sookmyung Women's University, South Korea*	**144**

🟦 METABOLOMICS IN HEALTH AND DISEASE

🟨 COMPUTATIONAL METABOLOMICS, STATISTICS & BIOINFORMATICS

★ AWARD WINNERS

Wednesday, June 19

Time	Session	Abstract #
8:30 a.m. – 9:30 a.m.	**Plenary Session 3** *Kazuki Saito, RIKEN Center For Sustainable Resource Science, Japan* Metabolomics revolutionizes phytochemical genomics	***Hall A***
10:15 a.m. – 12:00 p.m.	**Session 13. Metabolic Health** *Session Chairs: Natasa Giallourou and Thomas Moritz*	***Hall A***
10:15 a.m. – 10:45 a.m.	**13.1 KEYNOTE** Lipid profiling in children and adolescents with obesity *Cristina Legido Quigley, Kings College London, United Kingdom*	**452**
10:45 a.m. – 11:05 a.m.	**13.2** A Lipidomic based metabolic age score for assessing metabolic health and monitoring lifestyle interventions *Tingting Wang, Baker Heart and Diabetes Institute, Australia*	**145**
11:05 a.m. – 11:20 a.m.	**13.3** Plasma lipidomic associations with sex, age and adiposity in 1,955 Australian older adults from the Busselton Healthy Ageing Study *Alanah Grant–St James, Australian National Phenome Centre, Australia*	**142**
11:20 a.m. – 11:40 a.m.	**13.4** Dietary risk factors for visceral adiposity in multiethnic Asian population: An epidemiological and metabolomics study *Theresia Mina, Nanyang Technological University, Singapore*	**71**
11:40 a.m. – 12:00 p.m.	**13.5** Modeling Blood Metabolite Levels to Reduce Variability and Bias to Improve Biomarker Validation *Daniel Raftery, University Of Washington, United States*	**403**
10:15 a.m. – 12:00 p.m.	**Session 14. Machine Learning of Metabolics Data** *Session Chairs: Oliver Fiehn and Marvin Nathanael Iman*	***Hall D***
10:15 a.m. – 10:45 a.m.	**14.1 SESSION KEYNOTE** A Conversational AI-Agent for Accessible Mass Spectrometry Metabolomics Data Mining *Louis-Félix Nothias, Université Côte d'Azur, CNRS, ICN, France*	**320**
10:45 a.m. – 11:05 a.m.	**14.2** AI for High-throughput Metabolomics *Arzu Tugce Guler, Institute for Experiential AI At Northeastern Uni, United States*	**416**
11:05 a.m. – 11:20 a.m.	**14.3** AI-driven peak picking using convolutional neural networks and artificial chromatograms *Alice Limonciel, biocrates life sciences ag, Austria*	**372**
11:20 a.m. – 11:40 a.m.	**14.4** Integration of multi-assay liquid chromatography – mass spectrometry metabolomics data using multi-view machine learning *Lukas Kopecky, Imperial College London, United Kingdom*	**317**
11:40 a.m. – 12:00 p.m.	**14.5** Enhancing 2D J-Res NMR Spectra Resolution with J-RESRGAN: A Deep Learning Approach ★ *Yan Yan, Imperial College London, United Kingdom*	**193**

PLANTS, FOOD, ENVIRONMENT AND MICROBES

★ AWARD WINNERS

Wednesday, June 19

Time	Session	Abstract #
10:15 a.m. – 12:00 p.m.	**Session 15. Marine and Freshwater Metabolomics** *Session Chairs: Miyako Kusano and Millena Barros Santos*	***Hall E***
10:15 a.m. – 10:45 a.m.	**15.1 KEYNOTE** Evaluating environmental harm using a freshwater turtle model exposed to elevated Per- and poly-fluoroalkyl substances (PFAS) through omics-based ecosurveillance *David Beale, CSIRO, Australia*	**447**
10:45 a.m. – 11:05 a.m.	**15.2** Octadecanoids as emerging lipid mediators in coral-algal symbiosis ★ *Marina Tonetti Botana, Victoria University Of Wellington, New Zealand*	**323**
11:05 a.m. – 11:20 a.m.	**15.3** Temperature-induced metabolic adaptations in marine phytoplankton-parasite interactions ★ *Ruchicka Oniel, Mpi Fellow Group Plankton Community Interactions, Germany*	**168**
11:20 a.m. – 11:40 a.m.	**15.4** Identification of Toxicants in Baltic Sea Sediments with Aliivibrio fischeri Microtoxicity Assay and Non-Target Screening using Machine Learning for Prioritisation *Christine Gallampois, Umeå University, Sweden*	**118**
11:40 a.m. – 12:00 p.m.	**15.5** Understanding shrimp phenotypic responses to different environmental conditions using multi-omics approaches ★ *Umaporn Uawisetwathana, National Science And Technology Development Agency, Thailand*	**104**
12:20 p.m. – 1:20 p.m.	**Sponsor Lunch Presentations**	
SCIEX The Power of Precision	**AB SCIEX** The Pathway to Precision Metabolomics *Dr. Paul Baker, Senior Staff Scientist, SCIEX* *Prof. Hiroshi Tsugawa, Tokyo University of Agriculture and Technology* *Prof. Guowang Xu, Dalian Institute of Chemical Physics, Chinese Academy of Sciences*	***Hall D***
BRUKER	**Bruker** Advancing Analytical and Informatic Strategies for Comprehensive Untargeted Metabolomics *Prof. Zhengjiang Zhu, Principal Investigator, Director of Metabolomics Research Center, (IRCBC), (SIOC), Chinese Academy of Sciences* New NMR Applications in Clinical Research and Translation *Claire Wegner, Market Manager Clinical, Bruker BioSpin GmbH*	***Hall E***

🟦 METABOLOMICS IN HEALTH AND DISEASE
🟩 PLANTS, FOOD, ENVIRONMENT AND MICROBES

★ **AWARD WINNERS**

Wednesday, June 19

Time	Session	Abstract #
1:30 p.m. – 3:00 p.m.	**Session 16. Neurological Diseases** *Session Chairs: Su Chu and Thomas Vial*	***Hall A***
1:30 p.m. – 1:50 p.m.	**16.1** The metabolomic landscape of ADHD phenotypes in asthmatic children: an investigation of putative bioenergetic markers for asthma and ADHD overlap *Su Chu, Harvard Medical School, United States*	**413**
1:50 p.m. – 2:05 p.m.	**16.2** Unlocking Cognitive Impairment: Integrative Analysis Across Multiple Metabolomics and Lipidomics Platforms Reveals Promising Biomarkers for Diagnosis and Prognosis *Tereza Kacerova, University of Oxford, United Kingdom*	**129**
2:05 p.m. – 2:25 p.m.	**16.3** Elucidating the responsible cell- and genes for brain-specific acylated cerebroside ★ *Kuniyoshi Shimizu, Tokyo University of Agriculture and Technology, Japan*	**249**
2:25 p.m. – 2:40 p.m.	**16.4** Mass spectrometry imaging reveals region-specific alterations of brain lipids induced by parkinsonism and L-DOPA-induced dyskinesia *Ibrahim Kaya, Uppsala University, Sweden*	**108**
2:40 p.m. – 3:00 p.m.	**16.5** Multi-omics characterization of mouse models for Alzheimer's disease *Simone Zuffa, University of California San Diego, United States*	**81**
1:30 p.m. – 3:00 p.m.	**Session 17. Food Metabolomics** *Session Chairs: Eiichiro Fukusaki and Supaart Sirikantaramas*	***Hall D***
1:30 p.m. – 1:50 p.m.	**17.1** Food for Thought: Characterizing 500 Commonly Consumed Foods through Standardized Metabolomics for The Periodic Table of Food Initiative *Steven Watkins, Verso Biosciences, United States*	**405**
1:50 p.m. – 2:05 p.m.	**17.2** Metabolomics as a tool for authentication of edible insect-based food *Kateřina Šebelová, University of Chemistry and Technology, Czech Republic*	**387**
2:05 p.m. – 2:25 p.m.	**17.3** Uncovering Metabolic and Sensory Changes in Coffee Extracts via Ultrafiltration Membrane Processing *Mónica Cala, Universidad de Los Andes, Colombia*	**63**
2:25 p.m. – 2:40 p.m.	**17.4** Dynamics of Lipid Metabolism during Durian (Durio zibethinus L.) Ripening and Post-Harvest Using Lipidomics Analysis *Supakorn Potijun, Chulalongkorn University, Thailand*	**308**
2:40 p.m. – 3:00 p.m.	**17.5** The Germany Purity Law: detecting metabolite signatures of wheat, corn and rice in beer ★ *Stefan A. Pieczonka, Technical University of Munich (TUM), Germany*	**39**

★ AWARD WINNERS

Wednesday, June 19

Time	Session	Abstract #
1:30 p.m. – 3:00 p.m.	**Session 18. Liver Diseases** *Session Chairs: Nicholas Rattray and Aleš Kvasnička*	***Hall E***
1:30 p.m. – 1:50 p.m.	**18.1** Identification of Early Detection Biomarker Candidates From Global Urinary Metabolomic Profiles of Thai Intrahepatic Cholangiocarcinoma Patients *Yotsawat Pomyen, Chulabhorn Research Institute, Thailand*	**105**
1:50 p.m. – 2:05 p.m.	**18.2** Metabolomic Analysis Reveals Oxidative Stress Changes in NASH Patients with Isolated γ-Glutamyl Transferase Elevation ★ *Ju-Yu Chen, National Taiwan University, Taiwan*	**361**
2:05 p.m. – 2:25 p.m.	**18.3** Urine Metabolite Biomarkers of Alcohol-associated Liver Disease *Xiang Zhang, University of Louisville, United States*	**47**
2:25 p.m. – 2:40 p.m.	**18.4** Metabolome-microbiome Dynamics Following Cholangiocarcinoma Patient-derived Fecal Microbiota Transplantation and Oral Bile Reinfusion in Wistar Rat ★ *Jutarop Phetcharaburanin, Faculty of Medicine, Khon Kaen University, Thailand*	**383**
2:40 p.m. – 3:00 p.m.	**18.5** Lipidomics stratum corneum analysis links cutaneous biomarkers to metabolic-dysfunction associated steatotic liver disease *Xueheng Zhao, Cincinnati Children's Hospital Medical Center, United States*	**232**
3:30 p.m. – 5:10 p.m.	**Session 19. Maternal and Neonatal Health** *Session Chairs: Ryo Nakabayashi and Simone Zuffa*	***Hall A***
3:30 p.m. – 3:50 p.m.	**19.1** Characterization of the metabolome and microbiome landscape throughout pregnancy and early life. ★ *Milla F Brandao Gois, University Medical Center Groningen, Netherlands*	**362**
3:50 p.m. – 4:10 p.m.	**19.2** Development and application of an integrated workflow for nontargeted metabolomics and lipidomics: A comparative study of maternal and umbilical cord blood metabolic profiles ★ *Danyue Daisy Zhao, The Hong Kong Polytechnic University, Hong Kong*	**276**
4:10 p.m. – 4:30 p.m.	**19.3** Association of the serum lipoprotein profile with cardiometabolic risk in postpartum: Australian Cohort Study ★ *Reika Masuda, Murdoch University, Australia*	**146**
4:30 p.m. – 4:50 p.m.	**19.4** Survival of the littlest: Navigating sepsis diagnosis beyond inflammation in preterm neonates *Manchu Umarani Thangavelu, Leiden University, Netherlands*	**100**
4:50 p.m. – 5:10 p.m.	**19.5** Barriers and enablers to the effective implementation of (metabol)omics research in low- and middle-income countries: a qualitative study *Gerard Bryan Gonzales, Ghent University, Belgium*	**274**

🟨 COMPUTATIONAL METABOLOMICS, STATISTICS & BIOINFORMATICS

🟧 TECHNOLOGY ADVANCEMENTS

Wednesday, June 19

Time	Session	Abstract #
3:30 p.m. – 5:10 p.m.	**Session 20. Data Processing and Statistics** *Session Chairs: Stacey Reinke and David Wishart*	***Hall D***
3:30 p.m. – 3:50 p.m.	**20.1** MS-DIAL 5 multimodal mass spectrometry data mining unveils lipidome complexities *Hiroshi Tsugawa, Tokyo University of Agriculture and Technology, Japan*	**140**
3:50 p.m. – 4:10 p.m.	**20.2** Streamlining Integrative Mass Spectrometry Data Analysis in MZmine *Tomáš Pluskal, IOCB Prague, Czech Republic*	**99**
4:10 p.m. – 4:30 p.m.	**20.3** High-performance LC-MS metabolomics data processing using the Asari suite of tools *Joshua Mitchell, The Jackson Laboratory for Genomic Medicine, United States*	**191**
4:30 p.m. – 4:50 p.m.	**20.4** Standardizing nontargeted metabolomics and exposomics: The LC-BinBase environment *Oliver Fiehn, UC Davis, United States*	**327**
4:50 p.m. – 5:10 p.m.	**20.5** Metabolomics using variable selection ANOVA simultaneous component analysis (VASCA) and partial least squares-discriminant analysis (PLS-DA) to predict relapse and survival in metastatic colorectal cancer. *Caridad Díaz, Fundación Medina, Spain*	**119**
3:30 p.m. – 5:10 p.m.	**Session 21. Imaging and Fluxomics** *Session Chairs: Shuichi Shimma and Thusi Rupasinghe*	***Hall E***
3:30 p.m. – 3:50 p.m.	**21.1** Untargeted Pixel-by-Pixel Imaging of Metabolite Ratio Pairs as a Novel Tool for Biomedical Discovery in Mass Spectrometry Imaging *Qiuying Chen, Weill Cornell Medicine, United States*	**192**
3:50 p.m. – 4:10 p.m.	**21.2** A targeted mass spectrometry imaging workflow for spatial visualization of oxylipins in the airways *Craig Wheelock, Karolinska Institute, Sweden*	**359**
4:10 p.m. – 4:30 p.m.	**21.3** Implementation of SWATH data-indipendent isotopologues fragmentation pattern in 13C and 15N fluxomics: Why are we considering it imperative for the quantification of isotopologues? *Denise Drago, IRCCS San Raffaele Scientific Institute, Italy*	**222**
4:30 p.m. – 4:50 p.m.	**21.4** Tracing 13C6-Glucose metabolites by HRMS-MS/MS and two complementary UPLC separations: proof of concept for mouse heart tissue *Radmila Pavlovic, ProMeFa, Italia*	**226**
4:50 p.m. – 5:10 p.m.	**21.5** Mass spectrometrY-based Robust Isotopomer extrAction using myriaD (MYRIAD) for enhanced metabolic dynamics predictions. *Dries Verdegem, VIB – KU Leuven, Belgium*	**351**

🟦 **METABOLOMICS IN HEALTH AND DISEASE**
🟩 **PLANTS, FOOD, ENVIRONMENT AND MICROBES**

★ **AWARD WINNERS**

Thursday, June 20

Time	Session	Abstract #
8:30 a.m. – 9:30 a.m.	**Plenary Session 4** *Claudia Langenberg, Precision Healthcare University Research Institute, UK* From molecules to health records: utility of omics at population scale	***Hall A***
10:30 a.m. – 12:10 p.m.	**Session 22. Cancer** *Session Chairs: Julia Debik and Tomoyoshi Soga*	***Hall A***
10:30 a.m. – 11:00 a.m.	**22.1 SESSION KEYNOTE** Adiposity, metabolites, and endometrial cancer risk: Mendelian randomization and Observational analyses *Vanessa Tan, University Of Bristol, United Kingdom*	**84**
11:00 a.m. – 11:20 a.m.	**22.2** Exploring transcriptional and metabolic interactions in mutant isocitrate dehydrogenase 1 (IDH1) glioblastoma cells combining global RNA-seq and IC-MS-based metabolic profiling. *James McCullagh, University Of Oxford, United Kingdom*	**277**
11:20 a.m. – 11:35 a.m.	**22.3** Image-guided metabolomics and transcriptomics reveal tumour heterogeneity in luminal A and B human breast cancer beyond glucose tracer uptake *Sisi Deng, University of Tuebingen, WSIC – iFIT Exe Cluster, Germany*	**170**
11:35 a.m. – 11:55 a.m.	**22.4** A novel headspace thermal-desorption gas chromatography time-of-flight mass spectrometry workflow for early upper gastrointestinal cancer detection ★ *Philip Kwan Hung Leung, Imperial College London, United Kingdom*	**194**
11:55 a.m. – 12:10 p.m.	**22.5** Mapping the Terrain: Pancreatic ductal adenocarcinoma tumour influence on lung pre-metastatic niche explored through metabolomics and proteomics analysis ★ *Loic Mervant, The Francis Crick Institute, United Kingdom*	**179**
10:30 a.m. – 12:10 p.m.	**Session 23. Plant Metabolomics** *Session Chairs: Fidele Tugizimana and Akira Oikawa*	***Hall D***
10:30 a.m. – 11:00 a.m.	**23.1 KEYNOTE** Resilient berries – uncovering the mystery of botrytis reduction from shaking grapevines using metabolomics, lipidomics and mass spectrometry imaging *Farhana Pinu, New Zealand Institute For Plant And Food Research Ltd, New Zealand*	**426**
11:00 a.m. – 11:20 a.m.	**23.2** PiperNET: a multi-omics platform for the high-throughput elucidation of Piperaceae alkaloids' biosynthetic origin ★ *Tito Damiani, IOCB Prague, Czech Republic*	**131**
11:20 a.m. – 11:35 a.m.	**23.3** Cross species comparison of metabolomic profiles of Brassica plants under different stress conditions *Jemillie Madonna Samaniego De Leon, Nara Institute Of Science And Technology, Japan*	**341**
11:35 a.m. – 11:55 a.m.	**23.4** Activity based protein profiling (ABPP) for identification of molecular targets of isoliquiritigenin derived from Glycyrrhiza uralensis *Hina Sakai, Tokyo University of Agriculture and Technology, Japan*	**199**
11:55 a.m. – 12:10 p.m.	**23.5** Unraveling Brassica napus leaf metabolic diversity: leveraging machine learning for agronomic traits prediction *Millena Barros Santos, Bordeaux Metabolome-MetaboHUB, France*	**363**

TECHNOLOGY ADVANCEMENTS

★ **AWARD WINNERS**

Thursday, June 20

Time	Session	Abstract #
10:30 a.m. – 12:10 p.m.	**Session 24. Non-targeted and Semi-targeted Methods** *Session Chairs: Fumio Matsuda and Erica Forsberg*	*Hall E*
10:30 a.m. – 11:00 a.m.	**24.1 SESSION KEYNOTE** Combining metabolite standards cocktails with IDEOM v24 to enable routine semi-targeted metabolomics *Darren Creek, Monash University, Australia*	299
11:00 a.m. – 11:20 a.m.	**24.2** Advancing Ion Mobility–Mass Spectrometry to Improve Coverage and Accuracy in Untargeted Metabolomics *Zheng-Jiang Zhu, Shanghai Institute of Organic Chemistry, China*	70
11:20 a.m. – 11:35 a.m.	**24.3** Forward and Reverse Cosine Similarity Scoring During Real-Time Library Search for Triggering Additional Experiments on Indole Compounds *Brandon Bills, Thermo Fisher Scientific, United States*	102
11:35 a.m. – 11:55 a.m.	**24.4** Exploring novel endogenous metabolites using chemical labeling-based LC-MS *Pei Zhang, China Pharmaceutical University, China*	369
11:55 a.m. – 12:10 p.m.	**24.5** In-depth structural lipidomics using solid-phase extraction and electron activated dissociation-based tandem mass spectrometry techniques ★ *Manami Takeuchi, Tokyo University Of Agriculture And Technology, Japan*	285
12:25 p.m. – 1:25 p.m.	**Sponsor Lunch Presentations**	
SHIMADZU Excellence in Science	**Shimadzu Corporation** Empowering Discovery: Harnessing Comprehensive Targeted Metabolomics in a Metabolomics Core Facility *David De Souza, Facility Manager, Metabolomics Australia* High Throughput, High Spatially Resolved AP-MALDI MSI Pipeline *Vinod Narayana, Lead of Spatial Metabolomics and Lipidomics, Metabolomics Australia*	*Hall D*
Waters™	**Waters Corporation** Pushing the Boundaries of Science with Advanced Multi Reflecting Time-of-Flight (MRT) Technology *Jayne Kirk, Principal Consulting Product Manager, Waters Corporation* Assessing the Impact of Light Exercise Followed by a Stand-to-sit Postural Shift on Global Metabolic Profiles in Plasma *Liam M Heaney, Senior Lecturer, School of Sport, Exercise and Health Sciences, Loughborough University*	*Hall E*
1:30 p.m. – 3:15 p.m.	**Plenary Session 5 | Awards & Closing** *Yu Xia, Tsinghua University, China* Illuminating the dark lipidome with isomer-resolved mass spectrometry	*Hall A*