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
Computational Metabolomics, Statistics & Bioinformatics
Technology Advancements
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		

★ **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**

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** A simplified workflow for simultaneous quantification of hundreds of metabolites in a chemically complex biological extracts. *Vladimir Shulaev, University Of North Texas, United States*	**331**
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**

★ 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** Developing a panel of urinary biomarkers for the intake of foods commonly consumed in the UK *Juliet Vickar, Aberystwyth University, United Kingdom*	**293**
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-timepoints 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**

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**

★ **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 Metz*	***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**

★ **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** Multi-omics approaches for identification of HCC biomarkers in patients with liver cirrhosis *Habtom Ressom, Georgetown University, United States*	**410**
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** Bacille Calmette Guérin (BCG) and Hepatitis B Vaccine (HBV) Induce Distinct Changes in the Neonatal Plasma Metabolome *Joann Diray-Arce, Boston Children's Hospital, Harvard Medical School, United States*	**377**
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
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★ **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: Koel Chaudhury 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**

★ 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***