

## Metabolomics 2017 Detailed Program

\*Agenda subject to change.

### Monday 26 June

Time	Session	Location
8:45 - 10:15	Workshops	
10:15 - 10:30	Break	
10:30 - 12:00	Workshops	
13:15 - 14:00	Opening Ceremony	Great Hall 2
14:00 - 15:00	Plenary Speaker: Krishna Mahadevan Model-based Engineering of Metabolism	Great Hall 2
15:00 - 15:30	Tea and Coffee Break	Foyer
15:30 - 17:10	<b>Systems Biology Methods to Characterise Biological Systems</b> <i>Parallel Session 1A</i>	Room TBD
15:30 - 15:50	<b>Abstract 333</b> <b>A novel systemic approach to patient stratification</b> Maike Aurich, Luxembourg Centre for Systems Biomedicine, University of Luxembourg, Luxembourg	
15:50 - 16:10	<b>Abstract 171</b> <b>Laboratory Evolution Reveals Proximal and Distal Causation to Gene Loss</b> Douglas McCloskey, Center for Biosustainability, Denmark Technical University, Denmark	
16:10 - 16:30	<b>Abstract 477</b> <b>Comparative metabolomics of xylose-fermenting yeasts by UHPLC-MS/MS: effects of oxygen levels on fermentation performance</b> Patrícia Abdelnur, Embrapa Agroenergy, Brazil	
16:30 - 16:50	<b>Abstract 347</b> <b>An Integrative omics approach to disentangling the relationship between prenatal vitamin D exposure, 17q21 genetic variants, sphingolipid metabolism, and the development of asthma.</b> Jessica Lasky-Su, Brigham and Women's Hospital and Harvard Medical School, United States	
16:50 - 17:10	<b>Abstract 352</b> <b>MicrobiomeAnalyst - a web-based tool for comprehensive statistical, visual and functional analysis of microbiome data</b> JIANGUO XIA, McGill University, Canada	

<b>15:30 - 17:10</b>	<b>Model Organisms</b> <i>Parallel Session 1B</i>	Room TBD
15:30 - 15:50	<b>Abstract 148</b> <b>Actylcholine regulation after single pesticide exposure in relationship to developmental neurotoxicity, behavior and cognitive studies in mice</b> Pim Leonards, VU University, Netherlands	
15:50 - 16:10	<b>Abstract 420</b> <b>Using Metabolomics to Assess the Early Effects of Zinc and Boscalid On Estuarine Polychaete.</b> Georgia Sinclair, University of Melbourne, Australia	
16:10 - 16:30	<b>Abstract 44</b> <b>MS-based metabolomics reveals BDE47 associated neurometabolic changes</b> JI Fenfen, Hong Kong Baptist University, Hong Kong	
16:30 - 16:50	<b>Abstract 401</b> <b>Metabolomics study of triphenyl phosphate in earthworm Perionyx excavatus: biotransformation products and toxicity</b> Lei Wang, National University of Singapore, Singapore	
16:50 - 17:10	<b>Abstract 150</b> <b>The fate of technical-grade chlordane in mice fed a high-fat diet and its roles as a candidate obesogen</b> wentao zhu, China Agricultural University, China	
<b>15:30 - 17:10</b>	<b>Diabetes and Cardiovascular Disease</b> <i>Parallel Session 1C</i>	Room TBD
15:30 - 15:50	<b>Abstract 350</b> <b>Insufficient Sleep Alters Plasma Metabolites Linked to Insulin Resistance and Diabetes Risk</b> Christopher Depner, University of Colorado Boulder, United States	
15:50 - 16:10	<b>Abstract 279</b> <b>DMGV is a Novel Marker of Liver Fat and Predicts Future Development of Type 2 Diabetes</b> John O'Sullivan, Heart Research Institute, Australia	
16:10 - 16:30	<b>Abstract 341</b> <b>The metabolomic analysis of sequential hair segments reflected the metabolic changes of normal, small-for-gestational-age, and gestational diabetes mellitus affected pregnancies across the trimesters.</b> Ting-Li Han, Liggins Institute, The University of Auckland, Auckland, New Zealand, New Zealand	
16:30 - 16:50	<b>Abstract 237</b>	

**Molecular mechanisms of lung injury during cardiac surgery**

Raluca Maltesen, Aalborg University Hospital, Dep. of Anaesthesia and Intensive Care, Denmark

16:50 - 17:10

**Abstract 60**

**A non-targeted UHPLC-HRMS metabolomics pipeline for metabolite identification; application to cardiac remote ischemic preconditioning**

Nzoughet Kouassi Judith, Université d'Angers - UFR Santé - Institut MITOVASC, CNRS 6214, INSERM U1083, France

17:15 - 18:45

**Welcome Reception**  
**Poster Session 1**

Exhibit Hall

## Tuesday 27 June

Time	Session	Location
8:45 - 9:45	<b>Plenary Speaker: Hanne Bertram</b> Edibilomics	Great Hall 2
9:45 - 10:30	Break	Exhibit Hall
10:30 - 12:10	<b>The Staple Foods</b> <i>Parallel Session 2A</i>	Room TBD
10:30 - 10:50	<b>Abstract 111</b> <b>A multi-omics approach to understanding flavour-compound production in rice</b> Dara Daygon, The University of Queensland, Australia	
10:50 - 11:10	<b>Abstract 461</b> <b>Dietary whole grain modifies microbiota and enhances production of novel compounds associated with energy metabolism</b> Kati Hanhineva, University of Eastern Finland, Finland	
11:10 - 11:30	<b>Abstract 303</b> <b>GC/MS-based metabolomics approach for the discrimination of Indonesian specialty coffee</b> Sastia Putri, Department of Biotechnology, Graduate School of Engineering, Japan	
11:30 - 11:50	<b>Abstract 123</b> <b>Detection of Novel QTLs for Metabolomic and Agronomic traits in Tea (<i>Camellia sinensis</i>)</b> Robert Koech, University of Pretoria, South Africa	
11:50 - 12:10	<b>Abstract 272</b>	

**Milk lipidomics: what we know and what we don't**

zhiqian Liu, Agriculture Victoria, Australia

<b>10:30 - 12:10</b>	<b>Advances in Spatial Metabolomics</b> <i>Parallel Session 2B</i>	Room TBD
10:30 - 10:50	<b>Abstract 453</b> <b>Advancing Metabolomics through Imaging Mass Spectrometry and Direct Tissue Analysis</b> Richard Yost, University of Florida - Southeast Center for Integrated Metabolomics, United States	
10:50 - 11:10	<b>Abstract 273</b> <b>Enhanced Negative Mode Ion-less Matrices for Imaging Mass Spectrometry – Assessing MALDI Matrices for Metabolite Annotation and Spatial Metabolomics in Plant and Mammalian Systems</b> Berin Boughton, University of Melbourne, Australia	
11:10 - 11:30	<b>Abstract 222</b> <b>Contaminants removal from tissue samples using DESI Ion Mobility imaging</b> Vincen Wu, Imperial College London, United Kingdom	
11:30 - 11:50	<b>Abstract 317</b> <b>Application of optimised hierarchical agglomerative clustering for peak matching of large high resolution clinical mass spectrometry tissue imaging data</b> nazanin zounemat kermani, imperial college london, United Kingdom	
11:50 - 12:10	<b>Abstract 479</b> <b>3D Molecular Cartography of the Exposome and Metabolome of Fruits</b> Louis-Felix Nothias, CNRS / UC San Diego, France	
<b>10:30 - 12:10</b>	<b>Pregnancy, Infants and Children</b> <i>Parallel Session 2C</i>	Room TBD
10:30 - 10:50	<b>Abstract 169</b> <b>Correlation of a plasma metabolite score with duration of hypoxia: a piglet study</b> Julia Kuligowski, Health Research Institute La Fe, Spain	
10:50 - 11:10	<b>Abstract 342</b> <b>Pre-pregnancy maternal obesity can result in metabolic dysregulation and memory impairment in male offspring</b>	

Xiaobo Zhou, First Affiliated Hospital of Chongqing Medical University, China

- 11:10 - 11:30 **Abstract 244**  
**Rapid characterisation of the vaginal metabolome during pregnancy using desorption electrospray ionization (DESI) MS medical swab analysis**  
 Pamela Pruski, Imperial College London, United Kingdom
- 11:30 - 11:50 **Abstract 314**  
**Enrichment of Secondary Bile Acids associated with Food Allergy in Healthy Infant Cohort**  
 Yamini Virkud, Massachusetts General Hospital, United States
- 11:50 - 12:10 **Abstract 83**  
**Faecal and serum metabolomics in paediatric inflammatory bowel disease.**  
 Vidya Velagapudi, Institute for Molecular Medicine Finland FIMM, University of Helsinki, Finland

<b>12:10 - 13:30</b>	<b>Lunch</b> <b>Platinum Sponsor Presentations</b>	Exhibit Hall
<b>13:30 - 15:00</b>	<b>Advances in Statistics &amp; Machine Learning</b> <i>Parallel Session 3A</i>	Room TBD
13:30 - 14:00	<b>Keynote Speaker</b> <b>Novel methods for data generation and data integration in metabolomics</b> Johan Trygg, Umeå University, Sweden	
14:00 - 14:15	<b>Abstract 256</b> <b>When the microbiome meets the metabolome: A Framework for integrative longitudinal analysis</b> takoua jendoubi, School of public health, Imperial College London, United Kingdom	
14:15 - 14:30	<b>Abstract 309</b> <b>Multivariate modelling with unbiased variable selection</b> Carl Brunius, Chalmers University of Technology, Sweden	
14:30 - 14:45	<b>Abstract 217</b> <b>Feature extraction from high-dimensional metabolomics datasets using Knowledge Discovery by Accuracy Maximization (KODAMA)</b> Stefano Cacciatore, Imperial College, United Kingdom	
14:45 - 15:00	<b>Abstract 66</b>	

**A Graphical Cellular Dashboard for Analysis of Metabolomics Data**

Suzanne Paley, SRI International, United States

<b>13:30 - 15:00</b>	<b>Marine and Microbial Natural Products</b> <i>Parallel Session 3B</i>	Room TBD
13:30 - 14:00	<b>Abstract 143</b> <b>Identifying Marine Natural Products - Pitfalls and Progress</b> Mary Garson, The University of Queensland, Australia	
14:00 - 14:15	<b>Abstract 106</b> <b>Lipidome Remodeling at Sea: Viral Infection of a bloom forming Marine Algae Induces the Production of Highly Saturated Triacylglycerol</b> Sergey Malitsky, Weizmann Institute of Science, Israel	
14:15 - 14:30	<b>Abstract 57</b> <b>Metabolite Profiling of Red Sea Corals</b> Alejandra Ortega, KAUST, Saudi Arabia	
14:30 - 14:45	<b>Abstract 278</b> <b>Turning mould into gold: An exploration of mould metabolism to commercialize useful secondary metabolites</b> Kyle Van de Bittner, University of Canterbury, New Zealand	
14:45 - 15:00	<b>Abstract 157</b> <b>HSQC-TOCSY NMR profiling: making informed microbial strain selection for natural product discovery</b> Larissa Buedenbender, Environmental Futures Research Institute, School of Environment, Griffith UniversityGriffith University, Australia	
<b>13:30 - 15:00</b>	<b>Infectious Disease</b> <i>Parallel Session 3C</i>	Room TBD
13:30 - 14:00	<b>Abstract 324</b> <b>Metabolic reprogramming of macrophages exposed to Pseudomonas aeruginosa biofilm</b> Valerie Copie, Montana State University, United States	
14:00 - 14:15	<b>Abstract 366</b> <b>Exploring dormant genital tuberculosis associated infertility - 1H NMR based serum lipidomics approach</b> Koel Chaudhury, School of Medical Science and Technology, Indian Institute of Technology Kharagpur, India	
14:15 - 14:30	<b>Abstract 184</b>	

**Malaria parasite metabolism is supported by host derived nutrients obtained through RhopH2 mediated New Permeability Pathways**

Anubhav Srivastava, Monash Institute of Pharmaceutical Sciences, Australia

14:30 - 14:45 **Abstract 384**  
**Multi-omics analysis reveals the biochemical changes associated with artemisinin-resistant malaria parasites**  
 Darren Creek, Monash University, Australia

14:45 - 15:00 **Abstract 80**  
**Spatially resolved profiling of Polymyxin B induced acute kidney injury**  
 Andreas Dannhorn, Department of Surgery and Cancer, Sir Alexander Fleming Building, Imperial College, London SW7 2AZ, UK, United Kingdom

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**15:00 - 15:30** Break Exhibit Hall

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**15:30 - 17:00** **Nature's Apothecary** Room TBD  
*Parallel Session 4A*

15:30 - 16:00 **Keynote Speaker**  
**Strategies for TCMs Q-Marker discovery based on Chinmedomics**  
 Xijun Wang, Heilongjiang University of Chinese Medicine, China

16:00 - 16:15 **Abstract 156**  
**A multi-platform metabolomics approach to identify unique compounds present in Australian bush food**  
 Fe Calingacion, University of Queensland, Australia

16:15 - 16:30 **Abstract 89**  
**Comparative analysis of phytochemicals in the leaf extracts of *Pittosporum angustifolium* cultivars via LC-MS based plant metabolomics.**  
 ANUJA PATIL, SCHOOL OF PHARMACY, UNIVERSITY OF QUEENSLAND, Australia

16:30 - 16:45 **Abstract 263**  
**Deep metabolome annotation and the necessity of a thought experiment**  
 Gregory Genta-Jouve, University Paris Descartes, France

16:45 - 17:00 **Abstract 228**

**Metabolomics: The solution to assessing herbal medicine safety?**

Garth Maker, Murdoch University, Australia

<b>15:30 - 17:00</b>	<b>Frontiers in Lipidomics</b> <i>Parallel Session 4B</i>	Room TBD
15:30 - 16:00	<b>Abstract 425</b> <b>The use of ion mobility coupled with high resolution mass spectrometry to improve separation and identification of lipid biomarkers in metabolic diseases</b> Julian Griffin, University of Cambridge, United Kingdom	
16:00 - 16:15	<b>Abstract 212</b> <b>Exploring the use of ultra-high performance supercritical fluid chromatography mass spectrometry (UHPSFC-MS) for lipidomics applications</b> Joost Brandsma, University of Southampton, United Kingdom	
16:15 - 16:30	<b>Abstract 436</b> <b>Comprehensive High-Throughput Targeted Lipidomics</b> kevin huynh, Baker Heart and Diabetes Institute, Australia	
16:30 - 16:45	<b>Abstract 346</b> <b>Quantitative Lipidomics and Discovery Metabolomics Applied to Human Sebum</b> Elizaveta Freinkman, Metabolon, Inc., United States	
16:45 - 17:00	<b>Abstract 462</b> <b>Big fat back-track: mapping desaturase activity using ozone-induced dissociation mass spectrometry</b> Stephen Blanksby, Queensland University of Technology, Australia	
<b>15:30 - 17:00</b>	<b>Genome-scale Modelling &amp; Flux balance analysis</b> <i>Parallel Session 4C</i>	Room TBD
15:30 - 16:00	<b>Abstract 395</b> <b>Towards dynamic, genome-scale modeling that captures metabolite levels and regulation</b> Mark Styczynski, Georgia Institute of Technology, United States	
16:00 - 16:15	<b>Abstract 458</b> <b>Deciphering the metabolic responses to polymyxin killing in Acinetobacter baumannii ATCC 19606 by developing a high-quality genome-scale metabolic model</b>	



Yan Zhu, Monash Biomedicine Discovery Institute, Department of Microbiology, Faculty of Medicine, Nursing & Health Sciences, Monash University, Australia

- 16:15 - 16:30 **Abstract 328**  
**Dynamic flux modelling of adipocytes stimulated by insulin using <sup>13</sup>C-labelled metabolites**  
 Lake-Ee Quek, School of Mathematics and Statistics, The University of Sydney, Australia
- 16:30 - 16:45 **Abstract 282**  
**What is the relationship between intracellular and extracellular metabolites?**  
 Silas Villas-Boas, University of Auckland, New Zealand
- 16:45 - 17:00 **Abstract 387**  
**Enhancing tetanus toxin production through fermentation maps**  
 Esteban Marcellin, The University of Queensland, Australia

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**17:15 - 18:45** **Poster Session 2** Exhibit Hall

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**19:00 - 20:30** **EMN Reception**

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## Wednesday 28 June

Time	Session	Location
8:45 - 9:45	<b>Plenary Speaker: Anthony Carroll</b> Natural Products	Great Hall 2
9:45 - 10:30	Break	Exhibit Hall
<b>10:30 - 12:10</b>	<b>Natural Products and Metabolomics - Advancing Two Fields</b> <i>Parallel Session 5A</i>	Room TBD
10:30 - 10:50	<b>Abstract 190</b> <b>Comprehensive LC-MS/MS metabolomic profiling of fungal culture collections – insights into the chemical space of fungal secondary metabolites</b> Mark Sumarah, Agriculture and Agri-Food Canada, Canada	
10:50 - 11:10	<b>Abstract 302</b> <b>Defining the dark metabolism of the malaria parasite</b> Malcolm McConville, University of Melbourne, Australia	
11:10 - 11:30	<b>Abstract 367</b> <b>Development of Software for Efficient NMR Metabolomics Screening of Natural Products</b>	

Kimberly Colson, Bruker BioSpin, United States

11:30 - 11:50 **Abstract 62**  
**Differences in the biological architecture between visceral and subcutaneous adipose tissue revealed by transcriptomics and metabolomics**  
 Nasim Bararpour, University Center of Legal Medicine, Swaziland

11:50 - 12:10 **Abstract 104**  
**Next generation, 'standards-free' metabolite identification pipeline**  
 Ryan Renslow, Earth and Biological Sciences Directorate, Pacific Northwest National Laboratory (PNNL), Richland, WA, USA, United States

<b>10:30 - 12:10</b>	<b>Multi-omics / Systems Biology</b> <i>Parallel Session 5B</i>	Room TBD
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10:30 - 10:50 **Abstract 315**  
**A Systems Biology Approach to the Understanding of Asthma Severity through the Integration of Metabolomic, Transcriptomic and Epigenetic networks**  
 Rachel Kelly, Brigham and Women's Hospital Harvard Medical School, United States

10:50 - 11:10 **Abstract 178**  
**Intergenerational changes in faecal microbiome and metabolome in a C57BL/6J mouse colony**  
 Marten Snel, South Australian Health and Medical Research Institute, Australia

11:10 - 11:30 **Abstract 388**  
**Integrative Omics Approach Reveals Coordinate Regulation of Metabolites Glycosylation and Stress Hormones Biosynthesis by TT8 in Arabidopsis**  
 Shivshankar Umashankar, National University of Singapore, Singapore

11:30 - 11:50 **Abstract 154**  
**Multi-omics Analysis of Esophageal Adenocarcinoma: How Lipid Metabolism Affects Cancer Progression**  
 Jeffrey Molendijk, The University of Queensland Diamantina Institute, The University of Queensland, Brisbane, QLD, Australia, Australia

11:50 - 12:10 **Abstract 139**  
**Differential multi-fluid network sheds light on metabolic processes altered in end-stage renal disease**

Jonas Zierer, Helmholtz Zentrum München/King's College London,  
United Kingdom

<b>10:30 - 12:10</b>	<b>Cancer</b> <i>Parallel Session 5C</i>	Room TBD
10:30 - 10:50	<b>Abstract 48</b> <b>LC-MS-based metabolomics revealed SLC25A22 as an essential regulator in aspartate-derived amino acids and polyamines in KRAS-mutant colorectal cancer</b> Xiaona LI, State Key Laboratory of Environmental and Biological Analysis, Department of Chemistry, Hong Kong Baptist University, China	
10:50 - 11:10	<b>Abstract 146</b> <b>Metabolomic application of the Intelligent Knife (iKnife): Rapid Evaporative Ionisation Tandem Mass Spectrometry (REIMS/MS) for In-Vivo Metabolite and Tissue Identification in the Case of Breast Cancer</b> Zsolt Bodai, Imperial College London, United Kingdom	
11:10 - 11:30	<b>Abstract 129</b> <b>Spatial Imaging of Invasive ductal carcinoma specimens by Desorption Electrospray Ionisation Mass Spectrometry</b> DIPA GURUNG, Imperial College London, United Kingdom	
11:30 - 11:50	<b>Abstract 203</b> <b>Metabolic Reprogramming Induced by Retinoic Acid Ameliorates Desmoplasia in Pancreatic Cancer</b> Amrita Cheema, Georgetown University, United States	
11:50 - 12:10	<b>Abstract 478</b> <b>METABOLOMICS ANALYSIS DISTINGUISHES BETWEEN STAGES OF RENAL CELL CARCINOMA: A VALIDATION STUDY.</b> Oluyemi Falegan, University of Calgary, Canada	
<b>12:10 - 13:30</b>	<b>Lunch</b> <b>Platinum Sponsor Presentations</b>	Exhibit Hall
<b>13:30 - 15:00</b>	<b>Environment: Dipping into the Water</b> <i>Parallel Session 6A</i>	Room TBD
13:30 - 14:00	<b>Keynote Speaker</b> <b>Environmental Metabolomics</b> Jun Kikuchi, Riken, Japan	
14:00 - 14:15	<b>Abstract 149</b>	

**Metabolomics analysis of community interactions: the effect of species distributions and spatial heterogeneity on metabolic response.**

Jade O'Leary, Cardiff University, United Kingdom

14:15 - 14:30

**Abstract 271**

**Can metabolomics approaches be used to determine the impact of pollution in estuarine environments?**

Sara Long, University of Melbourne, Australia

14:30 - 14:45

**Abstract 86**

**Mapping carbon fate during coral bleaching: the application of 13C metabolomics**

Katie Hillyer, Victoria University of Wellington, New Zealand, New Zealand

14:45 - 15:00

**Abstract 427**

**Discrimination of natural and in vitro marine biofilms by LC-MS metabolomics**

Laurie Favre, MAPIEM, France

**13:30 - 15:00**

**New Tools in Natural Product Annotation**

Room TBD

*Parallel Session 6B*

13:30 - 14:00

**Abstract 313**

**Novel UHPLC-MS-SPE-NMR and UHPLC-timsTofMS/MS Tools for Higher-throughput, Confident Metabolite Identifications and to Address the Number One Grand Challenge of Metabolomics**

Lloyd Sumner, University of Missouri, United States

14:00 - 14:15

**Abstract 407**

**Ultrahigh-resolution metabolomics for heteroatom-containing specialized metabolites**

Ryo Nakabayashi, RIKEN Center for Sustainable Resource Science, Japan

14:15 - 14:30

**Abstract 258**

**CANOPUS - Comprehensive categorization of unknowns using tandem mass spectrometry**

Kai Dührkop, Friedrich-Schiller University, Jena, Germany

14:30 - 14:45

**Abstract 43**

**An automated, quantum-chemical in silico metabolite library engine for multidimensional NMR spectroscopy**

Jamie Dunn, Pacific Northwest National Laboratory, United States

14:45 - 15:00

**Abstract 292**

**Substance class annotation for long candidate lists in metabolite identification using structural ontologies**

Sarah Scharfenberg, Leibniz Institute of Plant Biochemistry, Germany

<b>13:30 - 15:00</b>	<b>Diet, Weight, and Physical Activity</b> <i>Parallel Session 6C</i>	Room TBD
13:30 - 14:00	<b>Abstract 474</b> <b>Systemic Impact of Roux-en-Y Gastric Bypass Surgery</b> JIA LI, Imperial College London, United Kingdom	
14:00 - 14:15	<b>Abstract 356</b> <b>How Blood Removal Affects Exercise Performance and the Plasma Metabolome</b> Nathan Lawler, Centre for Integrative Metabolomics & Computational Biology, School of Science, Edith Cowan University, Australia	
14:15 - 14:30	<b>Abstract 281</b> <b>Metabolomic analysis of the effects of a ten week high protein diet in older men</b> Amber Milan, Liggins Institute, University of Auckland, New Zealand	
14:30 - 14:45	<b>Abstract 82</b> <b>Analysis of the metabolomic responses to high protein meals in women at increased metabolic disease risk</b> Brenan Durainayagam, Liggins Institute, New Zealand	
14:45 - 15:00	<b>Abstract 241</b> <b>The effects of changing the liquid/solid content of an isoenergetic test meal on gastric emptying and the blood lipidome</b> Xuefei Li, Department of Biochemistry, University of Cambridge, United Kingdom	
<b>15:00 - 15:30</b>	Break	Exhibit Hall
<b>15:30 - 17:00</b>	<b>Wine, the Great Gift from Bacchus</b> <i>Parallel Session 7A</i>	Room TBD
15:30 - 16:00	<b>Keynote Speaker</b> <b>Metabolomics tools and approaches for characterising flavours, phenolics and quality markers in grapes and wine</b> Markus Herderich, The Australian Wine Research Institute, Australia	
16:00 - 16:15	<b>Abstract 128</b> <b>A metabolomic approach to determine the influence of grape ripening, cultivar, vineyard site and vintage on wine composition</b>	

Leigh Schmidtke, Charles Sturt University, National Wine and Grape Industry Centre, Australia

- 16:15 - 16:30 **Abstract 464**  
**Targeted metabolomics to provide insights into the role of trace sulfur compounds in wine aroma and quality**  
 Vilma Hysenaj, Metabolomics Australia, The Australian Wine Research Institute, PO BOX 147, Glen Osmond, 5064, Australia
- 16:30 - 16:45 **Abstract 163**  
**Using standardised drift-tube ion mobility to enhance non-targeted assessment of the wine metabolome**  
 Tim Causon, University of Natural Resources and Life Sciences, Austria
- 16:45 - 17:00 **Abstract 442**  
**A metabolomics approach to investigating red wine mouth-feel**  
 Emma Sherman, The New Zealand Institute for Plant & Food Research, New Zealand

<b>15:30 - 17:00</b>	<b>Metabolite Identification, Libraries, &amp; Cheminformatics</b> <i>Parallel Session 7B</i>	Room TBD
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- 15:30 - 16:00 **Abstract 264**  
**Identifying epimetabolites by mass spectrometry-based cheminformatics**  
 Hiroshi Tsugawa, RIKEN, Japan
- 16:00 - 16:15 **Abstract 268**  
**Curated open-access LC-Orbitrap-MS/MS spectral library of endogenous metabolites and lipids**  
 Prasad Phapale, EMBL, Germany
- 16:15 - 16:30 **Abstract 88**  
**The whole is easier than the parts: Improving molecular formula identification using Gibbs sampling on fragmentation trees**  
 Marcus Ludwig, Friedrich-Schiller-University Jena, Germany
- 16:30 - 16:45 **Abstract 301**  
**Automated metabolite substructure recommendation from unexplained spectra using pattern mining**  
 Aida Mrzic, University of Antwerp, Belgium
- 16:45 - 17:00 **Abstract 445**  
**Towards accessible, standard and reproducible Metabolomics**  
 Reza Salek, EMBL-EBI, United Kingdom

<b>15:30 - 17:00</b>	<b>Population-based Metabolomics Research</b> <i>Parallel Session 7C</i>	Room TBD
15:30 - 16:00	<b>Abstract 166</b> <b>Urinary metabolic profiles associated with 5-year changes in biomarkers of glucose homeostasis: an NMR spectroscopy based study</b> Nele Friedrich, Institute of Clinical Chemistry and Laboratory Medicine, University Medicine Greifswald, Greifswald, Germany, Germany	
16:00 - 16:15	<b>Abstract 289</b> <b>Plasma metabolites associated with type 2 diabetes in a Swedish population - a nested case-control study</b> LIN SHI, Department of Molecular Science, Swedish University of Agricultural Sciences, Sweden	
16:15 - 16:30	<b>Abstract 179</b> <b>Urinary metabolomics-based sub-phenotyping of a large-scale multi-omics asthma cohort identified tryptophan dysregulation associated with asthma</b> Stacey Reinke, Murdoch University, Australia	
16:30 - 16:45	<b>Abstract 239</b> <b>A robust analytical pipeline for high throughput molecular phenotyping of populations</b> Beatriz Jiménez, MRC-NIHR National Phenome Centre. Computational Systems Medicine. Imperial College London, United Kingdom	
16:45 - 17:00	<b>Abstract 230</b> <b>Metabolomics Approach in Tohoku Medical Megabank Project Prospective Cohort Studies</b> Seizo Koshiba, Tohoku University, Japan	
<b>17:15 - 18:45</b>	<b>Poster Session 3</b>	Exhibit Hall
<b>19:30 - 22:30</b>	<b>Conference Dinner</b>	

## Thursday 29 June

Time	Session	Location
<b>8:45 - 9:45</b>	<b>Plenary Speaker: Roy Goodacre</b> Lighting up the World of Metabolomics	Great Hall 2
<b>9:45 - 10:45</b>	<b>Poster Session 4</b>	Exhibit Hall

<b>10:45 - 12:15</b>	<b>Data Mining &amp; Computational Workflows</b> <i>Parallel Session 8A</i>	Room TBD
10:45 - 11:05	<b>Abstract 304</b> <b>Combining text mining and metabolic network algorithms to complement and interpret metabolic profiles</b> Fabien Jourdan, INRA-MetaboHub, France	
11:05 - 11:25	<b>Abstract 77</b> <b>MAIMS: a GAIMS alternative for the deconvolution of UDP-N-acetyl-D-glucosamine 13C mass isotopologue profiles</b> Dries Verdegem, Metabolomics Expertise Center - VIB / KU Leuven, Belgium	
11:25 - 11:45	<b>Abstract 444</b> <b>Identification and discrimination of sparse networks in metabolic systems</b> Lindy Rae, The University of New South Wales, Australia	
11:45 - 12:05	<b>Abstract 414</b> <b>Metabolomics on the cloud using workflows: the PhenoMeNal approach</b> Pablo Andres Moreno Cortez, EMBL-EBI The European Bioinformatics Institute, United Kingdom	
12:05 - 12:15	<b>Abstract 147</b> <b>Automated Real-Time Quality Control of LC-MS Metabolomics Data</b> Jan Stanstrup, Steno Diabetes Center Copenhagen, Denmark	
<b>10:45 - 12:15</b>	<b>Edibilomics</b> <i>Parallel Session 8B</i>	Room TBD
10:45 - 11:05	<b>Abstract 377</b> <b>Estimation of dietary intake; comparison of a dietary biomarker and a 4-day food diary</b> Lorraine Brennan, UCD Institute of Food and Health, Ireland	
11:05 - 11:25	<b>Abstract 108</b> <b>Demonstration of the utility of biomarkers for dietary intake assessment; proline betaine as an example</b> Helena Gibbons, University College Dublin, Ireland	
11:25 - 11:45	<b>Abstract 93</b> <b>MS-based Flavor Profiling of Okinawan Subtropical Plant Resources</b>	



Yonathan Asikin, Division of Biosphere Resource Science and Technology, Graduate School of Life and Environmental Sciences, University of Tsukuba, Japan

11:45 - 12:05 **Abstract 229**

**Inhibiting lipid oxidation using hydrophobic and hydrophilic natural antioxidants in an oil in water emulsion food system**

Sara Ghorbani Gorji, University of Queensland, Australia

12:05 - 12:15

**Abstract 220**

**Tomato juice consumption alters the human plasma metabolome**

Jessica Cooperstone, The Ohio State University, United States

**10:45 - 12:15**

**Metabolomics in Health and Disease I**

Room TBD

*Parallel Session 8C*

10:45 - 11:05

**Abstract 168**

**A combined metabolomics and lipidomics approach enables the stratification of acute-on-chronic liver failure patients according to their severity**

Francois Fenaille, CEA-INRA UMR 0496, Laboratoire d'Etude du Métabolisme des Médicaments, DRF/Institut Joliot/SPI, Université Paris Saclay, MetaboHUB, France

11:05 - 11:25

**Abstract 319**

**An integrated approach combining metabolomics, lipidomics and glycomics on plasma to highlight metabolism dysregulation in hepatic encephalopathy**

Pierre BARBIER SAINT HILAIRE, CEA, SPI, Laboratoire d'Etude du Métabolisme des Médicaments, MetaboHUB-IdF, Université Paris Saclay, 91191 Gif-sur-Yvette cedex, France, France

11:25 - 11:45

**Abstract 197**

**BIOMARKER DISCOVERY FOR HEPATITIS C PROGRESSION USING METABOLOMICS**

Heidi Spratt, University of Texas Medical Branch, United States

11:45 - 12:05

**Abstract 63**

**Investigation of drug-induced steatosis in HepaRG cells using untargeted LC-MS metabolomics**

Matthias Cuykx, Universiteit Antwerpen - Toxicological Centre, Belgium

12:05 - 12:15

**Abstract 381**

**Integrated omics profiling of NGLY1 deficiency disease**

Songjie Chen, Stanford University, United States

**12:15 - 13:45**      **Lunch**      Exhibit Hall

**Platinum Sponsor Presentations**

**13:45 - 15:15**      **Plants**      Room TBD

*Parallel Session 9A*

13:45 - 14:05      **Keynote Speaker**

**Challenging in Plant Metabolomics: How can we observe and interpret metabolomic data?**

Miyako Kusano, University of Tsukuba, Japan

14:05 - 14:25      **Abstract 71**

**An inducible system for anthocyanin accumulation in plants for application in green systems biology**

Robert Hall, Wageningen Plant Research, Netherlands

14:25 - 14:45      **Abstract 135**

**Geographic Mosaic of Metabolites in Purple Passionflower (*Passiflora incarnata*): Testing the Coevolutionary Hypothesis**

Nick Batora, University of Georgia, United States

14:45 - 15:05      **Abstract 69**

**Rice metabolomics: unravelling brown planthopper (BPH) resistance mechanism on BPH-resistant traits**

umaporn uawisetwathana, National Center for Genetic Engineering and Biotechnology, Thailand

15:05 - 15:15

**Abstract 447**

**A systems analysis of source-to-sink and metabolic regulatory mechanisms in tomato fruit development by narrowband-LED light treatments**

Atsushi Fukushima, RIKEN Center for Sustainable Resource Science, Japan

**13:45 - 15:15**      **Quantitative Metabolomics and Data Quality**      Room TBD

*Parallel Session 9B*

13:45 - 14:05      **Abstract 249**

**NMR Quantitates Whole Blood, Tissue and Even MS-Detected Metabolites**

Daniel Raftery, University of Washington, United States

14:05 - 14:25      **Abstract 127**

**Simultaneous Quantification of 124 Amino Metabolites in 22 Metabolic Pathways Using UHPLC-MS/MS**

Huiru Tang, Fudan University, China

14:25 - 14:45      **Abstract 172**

**Ion mobility–mass spectrometry based high-throughput metabolomics facilitates metabolite biomarker discovery in**  
Zhiwei Zhou, Chinese Academy of Sciences, China

14:45 - 15:05 **Abstract 473**  
**Towards reliable lipoprotein particle predictions from NMR spectra of human blood: Interlaboratory ring test validation of a**  
Bekzod Khakimov, Postdoc, Denmark

15:05 - 15:15 **Abstract 72**  
**Assessing Proficiency in Mass Spectrometric Lipid Measurement and Annotation using a NIST International Lipidomics Interlaboratory Comparison Exercise**  
Candice Ulmer, National Institute of Standards and Technology (NIST), United States

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<b>13:45 - 15:15</b>	<b>Metabolomics in Health and Disease II</b> <i>Parallel Session 9C</i>	Room TBD
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13:45 - 14:05 **Abstract 245**  
**Aiding diagnosis of rare disease: applications of mass spectrometry-based metabolomics in the Undiagnosed Diseases Network**  
Tom Metz, Pacific Northwest National Laboratory, United States

14:05 - 14:25 **Abstract 449**  
**Using U-13C glucose to determine the impairments in glucose metabolism in both acute and chronic epilepsy mouse models**  
Tanya McDonald, School of Biomedical Science, University of Queensland, Australia

14:25 - 14:45 **Abstract 134**  
**Metabonomic Study of Schizophrenia Using High-Resolution NMR Spectroscopy**  
Ute Marx, Hochschule Pforzheim, Germany

14:45 - 15:05 **Abstract 300**  
**LIPIDOMICS REVEALS CEREBROSPINAL-FLUID SIGNATURES OF ALS**  
BOCCA CINZIA, INSERMU930, France

15:05 - 15:15 **Abstract 466**  
**Plasma metabolite profiles allow diagnosis and disease course monitoring of primary progressive multiple sclerosis**  
Daniel Stoessel, Metabolomic Discoveries/ University of Potsdam, Germany

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**15:15 - 15:30 Gather in Great Hall 2 for Closing Plenary Session**

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<b>15:30 - 16:30</b>	<b>Plenary Speaker: Debra Meyer</b>	Great Hall 2
	Health and Medicine	

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<b>16:30 - 17:00</b>	<b>Closing Plenary Session</b>	Great Hall 2
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