

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	Systems Biology Methods to Characterise Biological Systems <i>Parallel Session 1A</i>	Meeting Room 1
15:30 - 15:50	Abstract 333 <i>A novel systemic approach to patient stratification</i> Maike Aurich, Luxembourg Centre for Systems Biomedicine, University of Luxembourg, Luxembourg	
15:50 - 16:10	Abstract 171 <i>Laboratory Evolution Reveals Proximal and Distal Causation to Gene Loss</i> Douglas McCloskey, Center for Biosustainability, Denmark Technical University, Denmark	
16:10 - 16:30	Abstract 477 <i>Comparative metabolomics of xylose-fermenting yeasts by UHPLC-MS/MS: effects of oxygen levels on fermentation performance</i> Patrícia Abdelnur, Embrapa Agroenergy, Brazil	
16:30 - 16:50	Abstract 347 <i>An Integrative omics approach to disentangling the relationship between prenatal vitamin D exposure, 17q21 genetic variants, sphingolipid metabolism, and the development of asthma.</i> Jessica Lasky-Su, Brigham and Women's Hospital and Harvard Medical School, United States	
16:50 - 17:10	Abstract 352 <i>MicrobiomeAnalyst - a web-based tool for comprehensive statistical, visual and functional analysis of microbiome data</i> JIANGUO XIA, McGill University, Canada	
15:30 - 17:10	Model Organisms <i>Parallel Session 1B</i>	Meeting Room 3
15:30 - 15:50	Abstract 148 <i>Acetylcholine regulation after single pesticide exposure in relationship to developmental neurotoxicity, behavior and cognitive studies in mice</i> Pim Leonards, VU University, Netherlands	

15:50 - 16:10	Abstract 420 <i>Using Metabolomics to Assess the Early Effects of Zinc and Boscalid On Estuarine Polychaete.</i> Georgia Sinclair, University of Melbourne, Australia	
16:10 - 16:30	Abstract 44 <i>MS-based metabolomics reveals BDE47 associated neurometabolic changes</i> JI Fenfen, Hong Kong Baptist University, Hong Kong	
16:30 - 16:50	Abstract 401 <i>Metabolomics study of triphenyl phosphate in earthworm <i>Perionyx excavatus</i>: biotransformation products and toxicity</i> Lei Wang, National University of Singapore, Singapore	
16:50 - 17:10	Abstract 150 <i>The fate of technical-grade chlordane in mice fed a high-fat diet and its roles as a candidate obesogen</i> wentao zhu, China Agricultural University, China	
15:30 - 17:10	Diabetes and Cardiovascular Disease <i>Parallel Session 1C</i>	Meeting Room 4
15:30 - 15:50	Abstract 350 <i>Insufficient Sleep Alters Plasma Metabolites Linked to Insulin Resistance and Diabetes Risk</i> Christopher Depner, University of Colorado Boulder, United States	
15:50 - 16:10	Abstract 279 <i>DMGV is a Novel Marker of Liver Fat and Predicts Future Development of Type 2 Diabetes</i> John O'Sullivan, Heart Research Institute, Australia	
16:10 - 16:30	Abstract 341 <i>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.</i> Ting-Li Han, Liggins Institute, The University of Auckland, Auckland, New Zealand, New Zealand	
16:30 - 16:50	Abstract 237 <i>Molecular mechanisms of lung injury during cardiac surgery</i> Raluca Maltesen, Aalborg University Hospital, Dep. of Anaesthesia and Intensive Care, Denmark	
16:50 - 17:10	Abstract 60 <i>A non-targeted UHPLC-HRMS metabolomics pipeline for metabolite identification; application to cardiac remote ischemic preconditioning</i> 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	Plenary Speaker: Hanne Bertram Edibilomics	Great Hall 2
9:45 - 10:30	Break	Exhibit Hall
10:30 - 12:10	The Staple Foods <i>Parallel Session 2A</i>	Meeting Room 1
10:30 - 10:50	Abstract 111 <i>A multi-omics approach to understanding flavour-compound production in rice</i> Dara Daygon, The University of Queensland, Australia	
10:50 - 11:10	Abstract 461 <i>Dietary whole grain modifies microbiota and enhances production of novel compounds associated with energy metabolism</i> Kati Hanhineva, University of Eastern Finland, Finland	
11:10 - 11:30	Abstract 303 <i>GC/MS-based metabolomics approach for the discrimination of Indonesian specialty coffee</i> Sastia Putri, Department of Biotechnology, Graduate School of Engineering, Japan	
11:30 - 11:50	Abstract 272 <i>Milk lipidomics: what we know and what we don't</i> Zhiqian Liu, Agriculture Victoria, Australia	
11:50 - 12:10	Round Table Discussion	
10:30 - 12:10	Advances in Spatial Metabolomics <i>Parallel Session 2B</i>	Meeting Room 3
10:30 - 10:50	Abstract 453 <i>Advancing Metabolomics through Imaging Mass Spectrometry and Direct Tissue Analysis</i> Richard Yost, University of Florida - Southeast Center for Integrated Metabolomics, United States	
10:50 - 11:10	Abstract 273 <i>Enhanced Negative Mode Ion-less Matrices for Imaging Mass Spectrometry – Assessing MALDI Matrices for Metabolite Annotation and Spatial Metabolomics in Plant and Mammalian Systems</i> Berin Boughton, University of Melbourne, Australia	
11:10 - 11:30	Abstract 222 <i>Contaminants removal from tissue samples using DESI Ion Mobility imaging</i> Vincen Wu, Imperial College London, United Kingdom	
11:30 - 11:50	Abstract 200	

	<i>MALDI Imaging of lipids and pharmaceuticals in human prostate cancer explants.</i> Paul Trim, SAHMRI, Australia	
11:50 - 12:10	Abstract 164 <i>NON-UNIFORM DISTRIBUTION OF METABOLITES IN ROOTS AS A RESULT OF A SHORT TERM SALINITY STRESS IN DIFFERING BARLEY CULTIVARS</i> Lenin Sarabia, University of Melbourne, Australia	
10:30 - 12:10	Pregnancy, Infants and Children <i>Parallel Session 2C</i>	Meeting Room 4
10:30 - 10:50	Abstract 169 <i>Correlation of a plasma metabolite score with duration of hypoxia: a piglet study</i> Julia Kuligowski, Health Research Institute La Fe, Spain	
10:50 - 11:10	Abstract 342 <i>Pre-pregnancy maternal obesity can result in metabolic dysregulation and memory impairment in male offspring</i> Xiaobo Zhou, First Affiliated Hospital of Chongqing Medical University, China	
11:10 - 11:30	Abstract 244 <i>Rapid characterisation of the vaginal metabolome during pregnancy using desorption electrospray ionization (DESI) MS medical swab analysis</i> Pamela Pruski, Imperial College London, United Kingdom	
11:30 - 11:50	Abstract 314 <i>Enrichment of Secondary Bile Acids associated with Food Allergy in Healthy Infant Cohort</i> Yamini Virkud, Massachusetts General Hospital, United States	
11:50 - 12:10	Abstract 83 <i>Faecal and serum metabolomics in paediatric inflammatory bowel disease.</i> Vidya Velagapudi, Institute for Molecular Medicine Finland FIMM, University of Helsinki, Finland	
12:10 - 13:30	Lunch Platinum Sponsor Presentations Agilent Technologies Shimadzu Australasia Waters Corporation	Exhibit Hall Meeting Room 1 Meeting Room 3 Meeting Room 4
13:30 - 15:00	Marine and Microbial Natural Products <i>Parallel Session 3A</i>	Meeting Room 1
13:30 - 14:00	Abstract 143 <i>Identifying Marine Natural Products - Pitfalls and Progress</i> Mary Garson, The University of Queensland, Australia	
14:00 - 14:15	Abstract 106	

Lipidome Remodeling at Sea: Viral Infection of a bloom forming Marine Algae Induces the Production of Highly Saturated Triacylglycerol

Sergey Malitsky, Weizmann Institute of Science, Israel

14:15 - 14:30

Abstract 57

Metabolite Profiling of Red Sea Corals

Alejandra Ortega, KAUST, Saudi Arabia

14:30 - 14:45

Abstract 278

Turning mould into gold: An exploration of mould metabolism to commercialize useful secondary metabolites

Kyle Van de Bittner, University of Canterbury, New Zealand

14:45 - 15:00

Abstract 157

HSQC-TOCSY NMR profiling: making informed microbial strain selection for natural product discovery

Larissa Buedenbender, Environmental Futures Research Institute, School of Environment, Griffith UniversityGriffith University, Australia

13:30 - 15:00

Advances in Statistics & Machine Learning

Meeting Room 3

Parallel Session 3B

13:30 - 14:00

Keynote Speaker

Novel methods for data generation and data integration in metabolomics

Johan Trygg, Umeå University, Sweden

14:00 - 14:15

Abstract 256

When the microbiome meets the metabolome: A Framework for integrative longitudinal analysis

Takoua Jendoubi, School of public health, Imperial College London, United Kingdom

14:15 - 14:30

Abstract 309

Multivariate modelling with unbiased variable selection

Carl Brunius, Chalmers University of Technology, Sweden

14:30 - 14:45

Abstract 217

Feature extraction from high-dimensional metabolomics datasets using Knowledge Discovery by Accuracy Maximization (KODAMA)

Stefano Cacciatore, Imperial College, United Kingdom

14:45 - 15:00

Abstract 66

A Graphical Cellular Dashboard for Analysis of Metabolomics Data

Suzanne Paley, SRI International, United States

13:30 - 15:00

Infectious Disease

Meeting Room 4

Parallel Session 3C

13:30 - 14:00

Abstract 384

	<i>Multi-omics analysis reveals the biochemical changes associated with artemisinin-resistant malaria parasites</i> Darren Creek, Monash University, Australia	
14:00 - 14:15	Abstract 366 <i>Exploring dormant genital tuberculosis associated infertility - 1H NMR based serum lipidomics approach</i> Koel Chaudhury, School of Medical Science and Technology, Indian Institute of Technology Kharagpur, India	
14:15 - 14:30	Abstract 184 <i>Malaria parasite metabolism is supported by host derived nutrients obtained through RhopH2 mediated New Permeability Pathways</i> Anubhav Srivastava, Monash Institute of Pharmaceutical Sciences, Australia	
14:30 - 14:45	Abstract 80 <i>Spatially resolved profiling of Polymyxin B induced acute kidney injury</i> Andreas Dannhorn, Department of Surgery and Cancer, Sir Alexander Fleming Building, Imperial College, London SW7 2AZ, UK, United Kingdom	
14:45 - 15:00	Round Table Discussion	
15:00 - 15:30	Break	Exhibit Hall
15:30 - 17:00	Genome-scale Modelling & Flux balance analysis <i>Parallel Session 4A</i>	Meeting Room 1
15:30 - 16:00	Abstract 395 <i>Towards dynamic, genome-scale modeling that captures metabolite levels and regulation</i> Mark Styczynski, Georgia Institute of Technology, United States	
16:00 - 16:15	Abstract 458 <i>Deciphering the metabolic responses to polymyxin killing in Acinetobacter baumannii ATCC 19606 by developing a high-quality genome-scale metabolic model</i> Yan Zhu, Monash Biomedicine Discovery Institute, Department of Microbiology, Faculty of Medicine, Nursing & Health Sciences, Monash University, Australia	
16:15 - 16:30	Abstract 328 <i>Dynamic flux modelling of adipocytes stimulated by insulin using 13C-labelled metabolites</i> Lake-Ee Quek, School of Mathematics and Statistics, The University of Sydney, Australia	
16:30 - 16:45	Abstract 282 <i>What is the relationship between intracellular and extracellular metabolites?</i> 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

15:30 - 17:00	Frontiers in Lipidomics	Meeting Room 3
<i>Parallel Session 4B</i>		
15:30 - 16:00	<p>Abstract 425 <i>The use of ion mobility coupled with high resolution mass spectrometry to improve separation and identification of lipid biomarkers in metabolic diseases</i> Julian Griffin, University of Cambridge, United Kingdom</p>	
16:00 - 16:15	<p>Abstract 212 <i>Exploring the use of ultra-high performance supercritical fluid chromatography mass spectrometry (UHPSFC-MS) for lipidomics applications</i> Joost Brandsma, University of Southampton, United Kingdom</p>	
16:15 - 16:30	<p>Abstract 436 <i>Comprehensive High-Throughput Targeted Lipidomics</i> kevin huynh, Baker Heart and Diabetes Institute, Australia</p>	
16:30 - 16:45	<p>Abstract 346 <i>Quantitative Lipidomics and Discovery Metabolomics Applied to Human Sebum</i> Elizaveta Freinkman, Metabolon, Inc., United States</p>	
16:45 - 17:00	<p>Round Table Discussion <i>Big fat back-track: mapping desaturase activity using ozone-induced dissociation mass spectrometry</i> Stephen Blanksby, Queensland University of Technology, Australia</p>	
15:30 - 17:00	Nature's Apothecary	Meeting Room 4
<i>Parallel Session 4C</i>		
15:30 - 16:00	<p>Abstract 228 <i>Metabolomics: The solution to assessing herbal medicine safety?</i> Garth Maker, Murdoch University, Australia</p>	
16:00 - 16:15	<p>Abstract 156 <i>A multi-platform metabolomics approach to identify unique compounds present in Australian bush food</i> Fe Calingacion, University of Queensland, Australia</p>	
16:15 - 16:30	<p>Abstract 89 <i>Comparative analysis of phytochemicals in the leaf extracts of Pittosporum angustifolium cultivars via LC-MS based plant metabolomics.</i> ANUJA PATIL, SCHOOL OF PHARMACY, UNIVERSITY OF QUEENSLAND, Australia</p>	
16:30 - 16:45	<p>Abstract 263 <i>Deep metabolome annotation and the necessity of a thought experiment</i> Gregory Genta-Jouve, University Paris Descartes, France</p>	
16:45 - 17:00	Round Table Discussion	

17:15 - 18:45	Poster Session 2	Exhibit Hall
19:00 - 20:30	EMN Reception	

Wednesday 28 June

Time	Session	Location
8:45 - 9:45	Plenary Speaker: Anthony Carroll Natural Products	Great Hall 2
9:45 - 10:30	Break	Exhibit Hall
10:30 - 12:10	Natural Products and Metabolomics - Advancing Two Fields <i>Parallel Session 5A</i>	Meeting Room 1
10:30 - 10:50	Abstract 190 <i>Comprehensive LC-MS/MS metabolomic profiling of fungal culture collections – insights into the chemical space of fungal secondary metabolites</i> Mark Sumarah, Agriculture and Agri-Food Canada, Canada	
10:50 - 11:10	Abstract 302 <i>Defining the dark metabolism of the malaria parasite</i> Malcolm McConville, University of Melbourne, Australia	
11:10 - 11:30	Abstract 367 <i>Development of Software for Efficient NMR Metabolomics Screening of Natural Products</i> Kimberly Colson, Bruker BioSpin, United States	
11:30 - 11:50	Abstract 62 <i>Differences in the biological architecture between visceral and subcutaneous adipose tissue revealed by transcriptomics and metabolomics</i> Nasim Bararpour, University Center of Legal Medicine, Switzerland	
11:50 - 12:10	Abstract 104 <i>Next generation, 'standards-free' metabolite identification pipeline</i> Ryan Renslow, Earth and Biological Sciences Directorate, Pacific Northwest National Laboratory (PNNL), Richland, WA, USA, United States	
10:30 - 12:10	Multi-omics / Systems Biology <i>Parallel Session 5B</i>	Meeting Room 3
10:30 - 10:50	Abstract 315 <i>A Systems Biology Approach to the Understanding of Asthma Severity through the Integration of Metabolomic, Transcriptomic and Epigenetic networks</i> 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

10:30 - 12:10

Cancer

Parallel Session 5C

Meeting Room 4

10:30 - 10:50

Abstract 48

LC-MS-based metabolomics revealed SLC25A22 as an essential regulator in aspartate-derived amino acids and polyamines in KRAS-mutant colorectal cancer

Xiaona LI, State Key Laboratory of Environmental and Biological Analysis, Department of Chemistry, Hong Kong Baptist University, China

10:50 - 11:10

Abstract 146

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

Zsolt Bodai, Imperial College London, United Kingdom

11:10 - 11:30

Abstract 129

Spatial Imaging of Invasive ductal carcinoma specimens by Desorption Electrospray Ionisation Mass Spectrometry

DIPA GURUNG, Imperial College London, United Kingdom

11:30 - 11:50

Abstract 203

Metabolic Reprogramming Induced by Retinoic Acid Ameliorates Desmoplasia in Pancreatic Cancer

Amrita Cheema, Georgetown University, United States

11:50 - 12:10

Abstract 172

Ion mobility–mass spectrometry based high-throughput metabolomics facilitates metabolite biomarker discovery in colorectal cancer

Zhiwei Zhou, Chinese Academy of Sciences, China

12:10 - 13:30	Lunch Platinum Sponsor Presentations Thermo Fisher Scientific Bruker Corporation SCIEX	Exhibit Hall Meeting Room 1 Meeting Room 3 Meeting Room 4
13:30 - 15:00	New Tools in Natural Product Annotation <i>Parallel Session 6A</i>	Meeting Room 1
13:30 - 14:00	Abstract 313 <i>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</i> Lloyd Sumner, University of Missouri, United States	
14:00 - 14:15	Abstract 407 <i>Ultrahigh-resolution metabolomics for heteroatom-containing specialized metabolites</i> Ryo Nakabayashi, RIKEN Center for Sustainable Resource Science, Japan	
14:15 - 14:30	Abstract 258 <i>CANOPUS - Comprehensive categorization of unknowns using tandem mass spectrometry</i> Kai Dührkop, Friedrich-Schiller University, Jena, Germany	
14:30 - 14:45	Abstract 43 <i>An automated, quantum-chemical in silico metabolite library engine for multidimensional NMR spectroscopy</i> Ryan Renslow, Earth and Biological Sciences Directorate, Pacific Northwest National Laboratory (PNNL), Richland, WA, USA, United States	
14:45 - 15:00	Abstract 292 <i>Substance class annotation for long candidate lists in metabolite identification using structural ontologies</i> Sarah Scharfenberg, Leibniz Institute of Plant Biochemistry, Germany	
13:30 - 15:00	Environment: Dipping into the Water <i>Parallel Session 6B</i>	Meeting Room 3
13:30 - 14:00	Keynote Speaker <i>Environmental Metabolomics</i> Jun Kikuchi, Riken, Japan	
14:00 - 14:15	Abstract 58 <i>LIPIDOMICS APPROACH TO IDENTIFY NOVEL SALINITY RESPONSE MECHANISUMS IN BARELY ROOTS</i> Thusitha Rupasinghe, Metabolomics Australia, Australia	
14:15 - 14:30	Abstract 271	

	<i>Can metabolomics approaches be used to determine the impact of pollution in estuarine environments?</i> Sara Long, University of Melbourne, Australia	
14:30 - 14:45	Abstract 86 <i>Mapping carbon fate during coral bleaching: the application of 13C metabolomics</i> Katie Hillyer, Victoria University of Wellington, New Zealand, New Zealand	
14:45 - 15:00	Abstract 427 <i>Discrimination of natural and in vitro marine biofilms by LC-MS metabolomics</i> Laurie Favre, MAPIEM, France	
13:30 - 15:00	Diet, Weight, and Physical Activity <i>Parallel Session 6C</i>	Meeting Room 4
13:30 - 14:00	Abstract 474 <i>Systemic Impact of Roux-en-Y Gastric Bypass Surgery</i> JIA LI, Imperial College London, United Kingdom	
14:00 - 14:15	Abstract 356 <i>How Blood Removal Affects Exercise Performance and the Plasma Metabolome</i> Nathan Lawler, Centre for Integrative Metabolomics & Computational Biology, School of Science, Edith Cowan University, Australia	
14:15 - 14:30	Abstract 281 <i>Metabolomic analysis of the effects of a ten week high protein diet in older men</i> Amber Milan, Liggins Institute, University of Auckland, New Zealand	
14:30 - 14:45	Abstract 82 <i>Analysis of the metabolomic responses to high protein meals in women at increased metabolic disease risk</i> Brenan Durainayagam, Liggins Institute, New Zealand	
14:45 - 15:00	Abstract 241 <i>The effects of changing the liquid/solid content of an isoenergetic test meal on gastric emptying and the blood lipidome</i> Xuefei Li, Department of Biochemistry, University of Cambridge, United Kingdom	
15:00 - 15:30	Break	Exhibit Hall
15:30 - 17:00	Metabolite Identification, Libraries, & Cheminformatics <i>Parallel Session 7A</i>	Meeting Room 1
15:30 - 16:00	Abstract 264 <i>Identifying epimetabolites by mass spectrometry-based cheminformatics</i> Hiroshi Tsugawa, RIKEN, Japan	
16:00 - 16:15	Abstract 268 <i>Curated open-access LC-Orbitrap-MS/MS spectral library of endogenous metabolites and lipids</i>	

16:15 - 16:30	Prasad Phapale, EMBL, Germany Abstract 88 <i>The whole is easier than the parts: Improving molecular formula identification using Gibbs sampling on fragmentation trees</i> Marcus Ludwig, Friedrich-Schiller-University Jena, Germany	
16:30 - 16:45	Abstract 301 <i>Automated metabolite substructure recommendation from unexplained spectra using pattern mining</i> Aida Mrzic, University of Antwerp, Belgium	
16:45 - 17:00	Abstract 445 <i>Towards accessible, standard and reproducible Metabolomics</i> Reza Salek, EMBL-EBI, United Kingdom	
15:30 - 17:00	Wine, the Great Gift from Bacchus <i>Parallel Session 7B</i>	Meeting Room 3
15:30 - 16:00	Keynote Speaker <i>Metabolomics tools and approaches for characterising flavours, phenolics and quality markers in grapes and wine</i> Markus Herderich, The Australian Wine Research Institute, Australia	
16:00 - 16:15	Abstract 128 <i>A metabolomic approach to determine the influence of grape ripening, cultivar, vineyard site and vintage on wine composition</i> Leigh Schmidtke, Charles Sturt University, National Wine and Grape Industry Centre, Australia	
16:15 - 16:30	Abstract 464 <i>Targeted metabolomics to provide insights into the role of trace sulfur compounds in wine aroma and quality</i> Vilma Hysenaj, Metabolomics Australia, The Australian Wine Research Institute, PO BOX 147, Glen Osmond, 5064, Australia	
16:30 - 16:45	Abstract 163 <i>Using standardised drift-tube ion mobility to enhance non-targeted assessment of the wine metabolome</i> Tim Causon, University of Natural Resources and Life Sciences, Austria	
16:45 - 17:00	Abstract 442 <i>A metabolomics approach to investigating red wine mouth-feel</i> Emma Sherman, The New Zealand Institute for Plant & Food Research, New Zealand	
15:30 - 17:00	Population-based Metabolomics Research <i>Parallel Session 7C</i>	Meeting Room 4
15:30 - 16:00	Abstract 166 <i>Urinary metabolic profiles associated with 5-year changes in biomarkers of glucose homeostasis: an NMR spectroscopy based study</i> Maik Pietzner, University Medicine Greifswald, Germany	
16:00 - 16:15	Abstract 289	

Plasma metabolites associated with type 2 diabetes in a Swedish population - a nested case-control study

LIN SHI, Department of Molecular Science, Swedish University of Agricultural Sciences, Sweden

16:15 - 16:30

Abstract 179

Urinary metabolomics-based sub-phenotyping of a large-scale multi-omics asthma cohort identified tryptophan dysregulation associated with asthma

Stacey Reinke, Murdoch University, Australia

16:30 - 16:45

Abstract 239

A robust analytical pipeline for high throughput molecular phenotyping of populations

Beatriz Jiménez, MRC-NIHR National Phenome Centre.

Computational Systems Medicine. Imperial College London, United Kingdom

16:45 - 17:00

Abstract 230

Metabolomics Approach in Tohoku Medical Megabank Project Prospective Cohort Studies

Seizo Koshiba, Tohoku University, Japan

17:15 - 18:45

Poster Session 3

Exhibit Hall

19:30 - 22:30

Conference Dinner

Plaza Ballroom

Thursday 29 June

Time	Session	Location
8:45 - 9:45	Plenary Speaker: Roy Goodacre Lighting up the World of Metabolomics	Great Hall 2
9:45 - 10:45	Poster Session 4	Exhibit Hall
10:45 - 12:15	Data Mining & Computational Workflows <i>Parallel Session 8A</i>	Meeting Room 1
10:45 - 11:05	Abstract 304 <i>Combining text mining and metabolic network algorithms to complement and interpret metabolic profiles</i> Fabien Jourdan, INRA-MetaboHub, France	
11:05 - 11:25	Abstract 77 <i>MAIMS: a GAIMS alternative for the deconvolution of UDP-N-acetyl-D-glucosamine 13C mass isotopologue profiles</i> Dries Verdegem, Metabolomics Expertise Center - VIB / KU Leuven, Belgium	
11:25 - 11:45	Abstract 444 <i>Identification and discrimination of sparse networks in metabolic systems</i> Lindy Rae, The University of New South Wales, Australia	

- 11:45 - 12:05 **Abstract 414**
Metabolomics on the cloud using workflows: the PhenoMeNal approach
 Pablo Andres Moreno Cortez, EMBL-EBI The European Bioinformatics Institute, United Kingdom
- 12:05 - 12:15 **Abstract 147**
Automated Real-Time Quality Control of LC-MS Metabolomics Data
 Jan Stanstrup, Steno Diabetes Center Copenhagen, Denmark

10:45 - 12:15	Edibilomics <i>Parallel Session 8B</i>	Meeting Room 3
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- 10:45 - 11:05 **Abstract 377**
Estimation of dietary intake; comparison of a dietary biomarker and a 4-day food diary
 Lorraine Brennan, UCD Institute of Food and Health, Ireland
- 11:05 - 11:25 **Abstract 108**
Demonstration of the utility of biomarkers for dietary intake assessment; proline betaine as an example
 Helena Gibbons, University College Dublin, Ireland
- 11:25 - 11:45 **Abstract 93**
MS-based Flavor Profiling of Okinawan Subtropical Plant Resources
 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 <i>Parallel Session 8C</i>	Meeting Room 4
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- 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 Presentation

Metabolon

Meeting Room 3

13:45 - 15:15

Quantitative Metabolomics and Data Quality

Meeting Room 1

Parallel Session 9A

13:45 - 14:15

Abstract 249

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

Daniel Raftery, University of Washington, United States

14:15 - 14:30

Abstract 198

High Throughput Lipid Identification and Quantification Using a Directed HRAM LC-MS-MS approach on a Modified Quadrupole-Orbitrap Mass Spectrometer

Reiko Kiyonami, Thermo Fisher Scientific, United States

14:30 - 14:45

Abstract 478

METABOLOMICS ANALYSIS DISTINGUISHES BETWEEN STAGES OF RENAL CELL CARCINOMA: A VALIDATION STUDY.

Oluyemi Falegan, University of Calgary, Canada

14:45 - 15:00

Abstract 473

Towards reliable lipoprotein particle predictions from NMR spectra of human blood: Interlaboratory ring test validation of a rigorously

Bekzod Khakimov, Postdoc, Denmark

15:00 - 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

13:45 - 15:15

Plants

Meeting Room 3

Parallel Session 9B

13:45 - 14:15

Keynote Speaker

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

Miyako Kusano, University of Tsukuba, Japan

14:15 - 14:30

Abstract 71

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

Robert Hall, Wageningen Plant Research, Netherlands

14:30 - 14:45

Abstract 135

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

Nick Batora, University of Georgia, United States

14:45 - 15:00

Abstract 69

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

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

15:00 - 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

Metabolomics in Health and Disease II

Meeting Room 4

Parallel Session 9C

13:45 - 14:15

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

14:15 - 14:30

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

14:30 - 14:45

Abstract 134

Metabonomic Study of Schizophrenia Using High-Resolution NMR Spectroscopy

Ute Marx, Hochschule Pforzheim, Germany

14:45 - 15:00

Abstract 300

LIPIDOMICS REVEALS CEREBROSPINAL-FLUID SIGNATURES OF ALS
BOCCA CINZIA, INSERMU930, France

Abstract 466

Plasma metabolite profiles allow diagnosis and disease course monitoring of primary progressive multiple sclerosis

15:00 - 15:15

Daniel Stoessel, Metabolomic Discoveries/ University of Potsdam, Germany

15:15 - 15:30

Gather in Great Hall 2 for Closing Plenary Session

15:30 - 16:30	Plenary Speaker: Huiru Tang <i>Simultaneous Quantification of 124 Amino Metabolites in 22 Metabolic Pathways Using UHPLC-MS/MS</i>	Great Hall 2
16:30 - 17:00	Closing Plenary Session	Great Hall 2
