

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 Perionyx excavatus: 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 123 <i>Detection of Novel QTLs for Metabolomic and Agronomic traits in Tea (Camellia sinensis)</i> Robert Koech, University of Pretoria, South Africa	
11:50 - 12:10	Abstract 272 <i>Milk lipidomics: what we know and what we don't</i> zhiqian Liu, Agriculture Victoria, Australia	
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>	

11:30 - 11:50	Vincen Wu, Imperial College London, United Kingdom Abstract 317 <i>Application of optimised hierarchical agglomerative clustering for peak matching of large high resolution clinical mass spectrometry tissue imaging data</i> nazanin zounemat kermani, imperial college london, United Kingdom	
11:50 - 12:10	Abstract 479 <i>3D Molecular Cartography of the Exposome and Metabolome of Fruits</i> Louis-Felix Nothias, CNRS / UC San Diego, France	
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	Advances in Statistics & Machine Learning <i>Parallel Session 3A</i>	Meeting Room 1
13:30 - 14:00	Keynote Speaker <i>Novel methods for data generation and data integration in metabolomics</i>	

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	Marine and Microbial Natural Products	Meeting Room 3
	<i>Parallel Session 3B</i>	

- 13:30 - 14:00 **Abstract 143**
Identifying Marine Natural Products - Pitfalls and Progress
 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 University Griffith University, Australia

13:30 - 15:00	Infectious Disease	Meeting Room 4
	<i>Parallel Session 3C</i>	

- 13:30 - 14:00 **Abstract 324**
Metabolic reprogramming of macrophages exposed to Pseudomonas aeruginosa biofilm
 Valerie Copie, Montana State University, United States

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 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 Andreas Dannhorn, Department of Surgery and Cancer, Sir Alexander Fleming Building, Imperial College, London SW7 2AZ, UK, United Kingdom	
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 Towards dynamic, genome-scale modeling that captures metabolite levels and regulation	
16:00 - 16:15	Abstract 458 Deciphering the metabolic responses to polymyxin killing in Acinetobacter baumannii ATCC 19606 by developing a high-quality genome-scale metabolic model 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 13C-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	

15:30 - 17:00	Frontiers in Lipidomics <i>Parallel Session 4B</i>	Meeting Room 3
15:30 - 16:00	Abstract 425 The use of ion mobility coupled with high resolution mass spectrometry to improve separation and identification of lipid biomarkers in metabolic diseases Julian Griffin, University of Cambridge, United Kingdom	
16:00 - 16:15	Abstract 212 Exploring the use of ultra-high performance supercritical fluid chromatography mass spectrometry (UHPSFC-MS) for lipidomics applications Joost Brandsma, University of Southampton, United Kingdom	
16:15 - 16:30	Abstract 436 Comprehensive High-Throughput Targeted Lipidomics kevin huynh, Baker Heart and Diabetes Institute, Australia	
16:30 - 16:45	Abstract 346 Quantitative Lipidomics and Discovery Metabolomics Applied to Human Sebum Elizaveta Freinkman, Metabolon, Inc., United States	
16:45 - 17:00	Abstract 462 Big fat back-track: mapping desaturase activity using ozone-induced dissociation mass spectrometry Stephen Blanksby, Queensland University of Technology, Australia	
15:30 - 17:00	Nature's Apothecary <i>Parallel Session 4C</i>	Meeting Room 4
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	

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 Comprehensive LC-MS/MS metabolomic profiling of fungal culture collections – insights into the chemical space of fungal secondary metabolites Mark Sumarah, Agriculture and Agri-Food Canada, Canada	
10:50 - 11:10	Abstract 302 Defining the dark metabolism of the malaria parasite Malcolm McConville, University of Melbourne, Australia	
11:10 - 11:30	Abstract 367 Development of Software for Efficient NMR Metabolomics Screening of Natural Products 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	
10:30 - 12:10	Multi-omics / Systems Biology <i>Parallel Session 5B</i>	Meeting Room 3
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

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 478

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

Oluyemi Falegan, University of Calgary, Canada

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	Environment: Dipping into the Water <i>Parallel Session 6A</i>	Meeting Room 1
13:30 - 14:00	Keynote Speaker Environmental Metabolomics Jun Kikuchi, Riken, Japan	
14:00 - 14:15	Abstract 149 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 <i>Parallel Session 6B</i>	Meeting Room 3
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	

14:30 - 14:45	Kai Dührkop, Friedrich-Schiller University, Jena, Germany Abstract 43 An automated, quantum-chemical in silico metabolite library engine for multidimensional NMR spectroscopy	
14:45 - 15:00	Jamie Dunn, Pacific Northwest National Laboratory, United States Abstract 292 Substance class annotation for long candidate lists in metabolite identification using structural ontologies	
13:30 - 15:00	Diet, Weight, and Physical Activity <i>Parallel Session 6C</i>	Meeting Room 4
13:30 - 14:00	Abstract 474 Systemic Impact of Roux-en-Y Gastric Bypass Surgery	
14:00 - 14:15	JIA LI, Imperial College London, United Kingdom Abstract 356 How Blood Removal Affects Exercise Performance and the Plasma Metabolome	
14:15 - 14:30	Nathan Lawler, Centre for Integrative Metabolomics & Computational Biology, School of Science, Edith Cowan University, Australia Abstract 281 Metabolomic analysis of the effects of a ten week high protein diet in older men	
14:30 - 14:45	Amber Milan, Liggins Institute, University of Auckland, New Zealand Abstract 82 Analysis of the metabolomic responses to high protein meals in women at increased metabolic disease risk	
14:45 - 15:00	Brenan Durainayagam, Liggins Institute, New Zealand Abstract 241 The effects of changing the liquid/solid content of an isoenergetic test meal on gastric emptying and the blood lipidome	
15:00 - 15:30	Break	Exhibit Hall
15:30 - 17:00	Wine, the Great Gift from Bacchus <i>Parallel Session 7A</i>	Meeting Room 1
15:30 - 16:00	Keynote Speaker Metabolomics tools and approaches for characterising flavours, phenolics and quality markers in grapes and wine	
16:00 - 16:15	Markus Herderich, The Australian Wine Research Institute, Australia Abstract 128 A metabolomic approach to determine the influence of grape ripening, cultivar, vineyard site and vintage on wine composition	
	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 Wilma 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	
15:30 - 17:00	Metabolite Identification, Libraries, & Cheminformatics <i>Parallel Session 7B</i>	Meeting Room 3
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	
15:30 - 17:00	Population-based Metabolomics Research <i>Parallel Session 7C</i>	Meeting Room 4
15:30 - 16:00	Abstract 166 Urinary metabolic profiles associated with 5-year changes in biomarkers of glucose homeostasis: an NMR spectroscopy based study Nele Friedrich, Institute of Clinical Chemistry and Laboratory Medicine, University Medicine Greifswald, Greifswald, Germany, 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 Combining text mining and metabolic network algorithms to complement and interpret metabolic profiles Fabien Jourdan, INRA-MetaboHub, France	
11:05 - 11:25	Abstract 77 MAIMS: a GAIMS alternative for the deconvolution of UDP-N-acetyl-D-glucosamine 13C mass isotopologue profiles Dries Verdegem, Metabolomics Expertise Center - VIB / KU Leuven, Belgium	
11:25 - 11:45	Abstract 444 Identification and discrimination of sparse networks in metabolic systems 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 Meeting Room 3

Parallel Session 8B

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 Meeting Room 4

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

11:25 - 11:45	<p>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</p> <p>Abstract 197 BIOMARKER DISCOVERY FOR HEPATITIS C PROGRESSION USING METABOLOMICS Heidi Spratt, University of Texas Medical Branch, United States</p>	
11:45 - 12:05	<p>Abstract 63 Investigation of drug-induced steatosis in HepaRG cells using untargeted LC-MS metabolomics Matthias Cuykx, Universiteit Antwerpen - Toxicological Centre, Belgium</p>	
12:05 - 12:15	<p>Abstract 381 Integrated omics profiling of NGLY1 deficiency disease Songjie Chen, Stanford University, United States</p>	
12:15 - 13:45	<p>Lunch Platinum Sponsor Presentation Metabolon</p>	<p>Exhibit Hall Meeting Room 3</p>
13:45 - 15:15	<p>Plants <i>Parallel Session 9A</i></p>	Meeting Room 1
13:45 - 14:05	<p>Keynote Speaker Challenging in Plant Metabolomics: How can we observe and interpret metabolomic data? Miyako Kusano, University of Tsukuba, Japan</p>	
14:05 - 14:25	<p>Abstract 71 An inducible system for anthocyanin accumulation in plants for application in green systems biology Robert Hall, Wageningen Plant Research, Netherlands</p>	
14:25 - 14:45	<p>Abstract 135 Geographic Mosaic of Metabolites in Purple Passionflower (<i>Passiflora incarnata</i>): Testing the Coevolutionary Hypothesis Nick Batora, University of Georgia, United States</p>	
14:45 - 15:05	<p>Abstract 69 Rice metabolomics: unravelling brown planthopper (BPH) resistance mechanism on BPH-resistant traits umaporn uawisetwathana, National Center for Genetic Engineering and Biotechnology, Thailand</p>	
15:05 - 15:15	<p>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</p>	
13:45 - 15:15	<p>Quantitative Metabolomics and Data Quality <i>Parallel Session 9B</i></p>	Meeting Room 3
13:45 - 14:05	<p>Abstract 249</p>	

	<p>NMR Quantitates Whole Blood, Tissue and Even MS-Detected Metabolites Daniel Raftery, University of Washington, United States</p>	
14:05 - 14:25	<p>Abstract 127 Simultaneous Quantification of 124 Amino Metabolites in 22 Metabolic Pathways Using UHPLC-MS/MS Huiru Tang, Fudan University, China</p>	
14:25 - 14:45	<p>Abstract 172 Ion mobility–mass spectrometry based high-throughput metabolomics facilitates metabolite biomarker discovery in Zhiwei Zhou, Chinese Academy of Sciences, China</p>	
14:45 - 15:05	<p>Abstract 473 Towards reliable lipoprotein particle predictions from NMR spectra of human blood: Interlaboratory ring test validation of a Bekzod Khakimov, Postdoc, Denmark</p>	
15:05 - 15:15	<p>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</p>	
13:45 - 15:15	Metabolomics in Health and Disease II	Meeting Room 4
	<i>Parallel Session 9C</i>	
13:45 - 14:05	<p>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</p>	
14:05 - 14:25	<p>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</p>	
14:25 - 14:45	<p>Abstract 134 Metabonomic Study of Schizophrenia Using High-Resolution NMR Spectroscopy Ute Marx, Hochschule Pforzheim, Germany</p>	
14:45 - 15:05	<p>Abstract 300 LIPIDOMICS REVEALS CEREBROSPINAL-FLUID SIGNATURES OF ALS BOCCA CINZIA, INSERMU930, France</p>	
15:05 - 15:15	<p>Abstract 466 Plasma metabolite profiles allow diagnosis and disease course monitoring of primary progressive multiple sclerosis Daniel Stoessel, Metabolomic Discoveries/ University of Potsdam, Germany</p>	
15:15 - 15:30	Gather in Great Hall 2 for Closing Plenary Session	
15:30 - 16:30	Plenary Speaker: Debra Meyer	Great Hall 2

Health and Medicine

16:30 - 17:00	Closing Plenary Session	Great Hall 2
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