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

15:50 - 16:10	**Abstract 420** *Using Metabolomics to Assess the Early Effects of Zinc and Boscalid On Estuarine Polychaete.* Georgia Sinclair, University of Melbourne, Australia	
16:10 - 16:30	**Abstract 44** *MS-based metabolomics reveals BDE47 associated neurometabolic changes* JI Fenfen, Hong Kong Baptist University, Hong Kong	
16:30 - 16:50	**Abstract 401** *Metabolomics study of triphenyl phosphate in earthworm Perionyx excavatus: biotransformation products and toxicity* Lei Wang, National University of Singapore, Singapore	
16:50 - 17:10	**Abstract 150** *The fate of technical-grade chlordane in mice fed a high-fat diet and its roles as a candidate obesogen* wentao zhu, China Agricultural University, China	
15:30 - 17:10	**Diabetes and Cardiovascular Disease** *Parallel Session 1C*	Meeting Room 4
15:30 - 15:50	**Abstract 350** *Insufficient Sleep Alters Plasma Metabolites Linked to Insulin Resistance and Diabetes Risk* Christopher Depner, University of Colorado Boulder, United States	
15:50 - 16:10	**Abstract 279** *DMGV is a Novel Marker of Liver Fat and Predicts Future Development of Type 2 Diabetes* John O'Sullivan, Heart Research Institute, Australia	
16:10 - 16:30	**Abstract 341** *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.* Ting-Li Han, Liggins Institute, The University of Auckland, Auckland, New Zealand, New Zealand	
16:30 - 16:50	**Abstract 237** *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	**Plenary Speaker: Hanne Bertram** Edibilomics	Great Hall 2
9:45 - 10:30	Break	Exhibit Hall
10:30 - 12:10	**The Staple Foods** *Parallel Session 2A*	Meeting Room 1
10:30 - 10:50	**Abstract 111** *A muti-omics approach to understanding flavour-compound production in rice* Dara Daygon, The University of Queensland, Australia	
10:50 - 11:10	**Abstract 461** *Dietary whole grain modifies microbiota and enhances production of novel compounds associated with energy metabolism* Kati Hanhineva, University of Eastern Finland, Finland	
11:10 - 11:30	**Abstract 303** *GC/MS-based metabolomics approach for the discrimination of Indonesian specialty coffee* Sastia Putri, Department of Biotechnology, Graduate School of Engineering, Japan	
11:30 - 11:50	**Abstract 123** *Detection of Novel QTLs for Metabolomic and Agronomic traits in Tea (Camellia sinensis)* Robert Koech, University of Pretoria, South Africa	
11:50 - 12:10	**Abstract 272** *Milk lipidomics: what we know and what we don't* zhiqian Liu, Agriculture Victoria, Australia	
10:30 - 12:10	**Advances is Spatial Metabolomics** *Parallel Session 2B*	Meeting Room 3
10:30 - 10:50	**Abstract 453** *Advancing Metabolomics through Imaging Mass Spectrometry and Direct Tissue Analysis* Richard Yost, University of Florida - Southeast Center for Integrated Metabolomics, United States	
10:50 - 11:10	**Abstract 273** *Enhanced Negative Mode Ion-less Matrices for Imaging Mass Spectrometry – Assessing MALDI Matrices for Metabolite Annotation and Spatial Metabolomics in Plant and Mammalian Systems* Berin Boughton, University of Melbourne, Australia	
11:10 - 11:30	**Abstract 222** *Contaminants removal from tissue samples using DESI Ion Mobility imaging*	

	Vincen Wu, Imperial College London, United Kingdom	
11:30 - 11:50	**Abstract 200** *MALDI Imaging of lipids and pharmaceuticals in human prostate cancer explants.* Paul Trim, SAHMRI, Australia	
11:50 - 12:10	**Abstract 164** *NON-UNIFORM DISTRIBUTION OF METABOLITES IN ROOTS AS A RESULT OF A SHORT TERM SALINITY STRESS IN DIFFERING BARLEY CULTIVARS* Lenin Sarabia, University of Melbourne, Australia	
10:30 - 12:10	**Pregnancy, Infants and Children** *Parallel Session 2C*	Meeting Room 4
10:30 - 10:50	**Abstract 169** *Correlation of a plasma metabolite score with duration of hypoxia: a piglet study* Julia Kuligowski, Health Research Institute La Fe, Spain	
10:50 - 11:10	**Abstract 342** *Pre-pregnancy maternal obesity can result in metabolic dysregulation and memory impairment in male offspring* 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	
12:10 - 13:30	**Lunch**	Exhibit Hall
	Platinum Sponsor Presentations	
	Agilent Technologies	Meeting Room 1
	Shimadzu Australasia	Meeting Room 3
	Waters Corporation	Meeting Room 4
13:30 - 15:00	**Advances in Statistics & Machine Learning** *Parallel Session 3A*	Meeting Room 1
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 **Marine and Microbial Natural Products** Meeting Room 3
Parallel Session 3B

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 UniversityGriffith University, Australia

13:30 - 15:00 **Infectious Disease** Meeting Room 4
Parallel Session 3C

13:30 - 14:00 **Abstract 384**
Multi-omics analysis reveals the biochemical changes associated with artemisinin-resistant malaria parasites
Darren Creek, Monash University, Australia

14:00 - 14:15	**Abstract 366** *Exploring dormant genital tuberculosis associated infertility - 1H NMR based serum lipidomics approach* 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** *Parallel Session 4A*	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** *Parallel Session 4B*	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** *Parallel Session 4C*	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** *Parallel Session 5A*	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, Switzerland	
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** *Parallel Session 5B*	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 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	**Environment: Dipping into the Water** *Parallel Session 6A*	Meeting Room 1
13:30 - 14:00	**Keynote Speaker** *Environmental Metabolomics* Jun Kikuchi, Riken, Japan	
14:00 - 14:15	**Abstract 58** *LIPIDOMICS APROACH TO IDENTIFY NOVEL SALINITY RESPONSE MECHANISUMS IN BARELY ROOTS* Thusitha Rupasinghe, Metabolomics Australia, Australia	
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** *Parallel Session 6B*	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*	

	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	
13:30 - 15:00	**Diet, Weight, and Physical Activity** *Parallel Session 6C*	Meeting Room 4
13:30 - 14:00	**Abstract 474** *Systemic Impact of Roux-en-Y Gastric Bypass Surgery* JIA LI, Imperial College London, United Kingdom	
14:00 - 14:15	**Abstract 356** *How Blood Removal Affects Exercise Performance and the Plasma Metabolome* Nathan Lawler, Centre for Integrative Metabolomics & Computational Biology, School of Science, Edith Cowan University, Australia	
14:15 - 14:30	**Abstract 281** *Metabolomic analysis of the effects of a ten week high protein diet in older men* Amber Milan, Liggins Institute, University of Auckland, New Zealand	
14:30 - 14:45	**Abstract 82** *Analysis of the metabolomic responses to high protein meals in women at increased metabolic disease risk* Brenan Durainayagam, Liggins Institute, New Zealand	
14:45 - 15:00	**Abstract 241** *The effects of changing the liquid/solid content of an isoenergetic test meal on gastric emptying and the blood lipidome* Xuefei Li, Department of Biochemistry, University of Cambridge, United Kingdom	
15:00 - 15:30	Break	Exhibit Hall
15:30 - 17:00	**Wine, the Great Gift from Bacchus** *Parallel Session 7A*	Meeting Room 1
15:30 - 16:00	**Keynote Speaker** *Metabolomics tools and approaches for characterising flavours, phenolics and quality markers in grapes and wine* Markus Herderich, The Australian Wine Research Institute, Australia	
16:00 - 16:15	**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* 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	
15:30 - 17:00	**Metabolite Identification, Libraries, & Cheminformatics** *Parallel Session 7B*	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** *Parallel Session 7C*	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** *Parallel Session 8A*	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** *Parallel Session 8B*	Meeting Room 3
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** *Parallel Session 8C*	Meeting Room 4
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** **Platinum Sponsor Presentation** Metabolon	Exhibit Hall Meeting Room 3
13:45 - 15:15	**Plants** *Parallel Session 9A*	Meeting Room 1
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	**Quantitative Metabolomics and Data Quality** *Parallel Session 9B*	Meeting Room 3
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 127** *Simultaneous Quantification of 124 Amino Metabolites in 22 Metabolic Pathways Using UHPLC-MS/MS* Huiru Tang, Fudan University, China	
14:30 - 14:45	**Abstract 478** *Ion mobility–mass spectrometry based high-throughput metabolomics facilitates metabolite biomarker discovery in* Zhiwei Zhou, Chinese Academy of Sciences, China	
14:45 - 15:00	**Abstract 473** *METABOLOMICS ANALYSIS DISTINGUISHES BETWEEN STAGES OF RENAL CELL CARCINOMA: A VALIDATION STUDY.* Oluyemi Falegan, University of Calgary, Canada	
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	**Metabolomics in Health and Disease II** *Parallel Session 9C*	Meeting Room 4
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	
15:00 - 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	
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