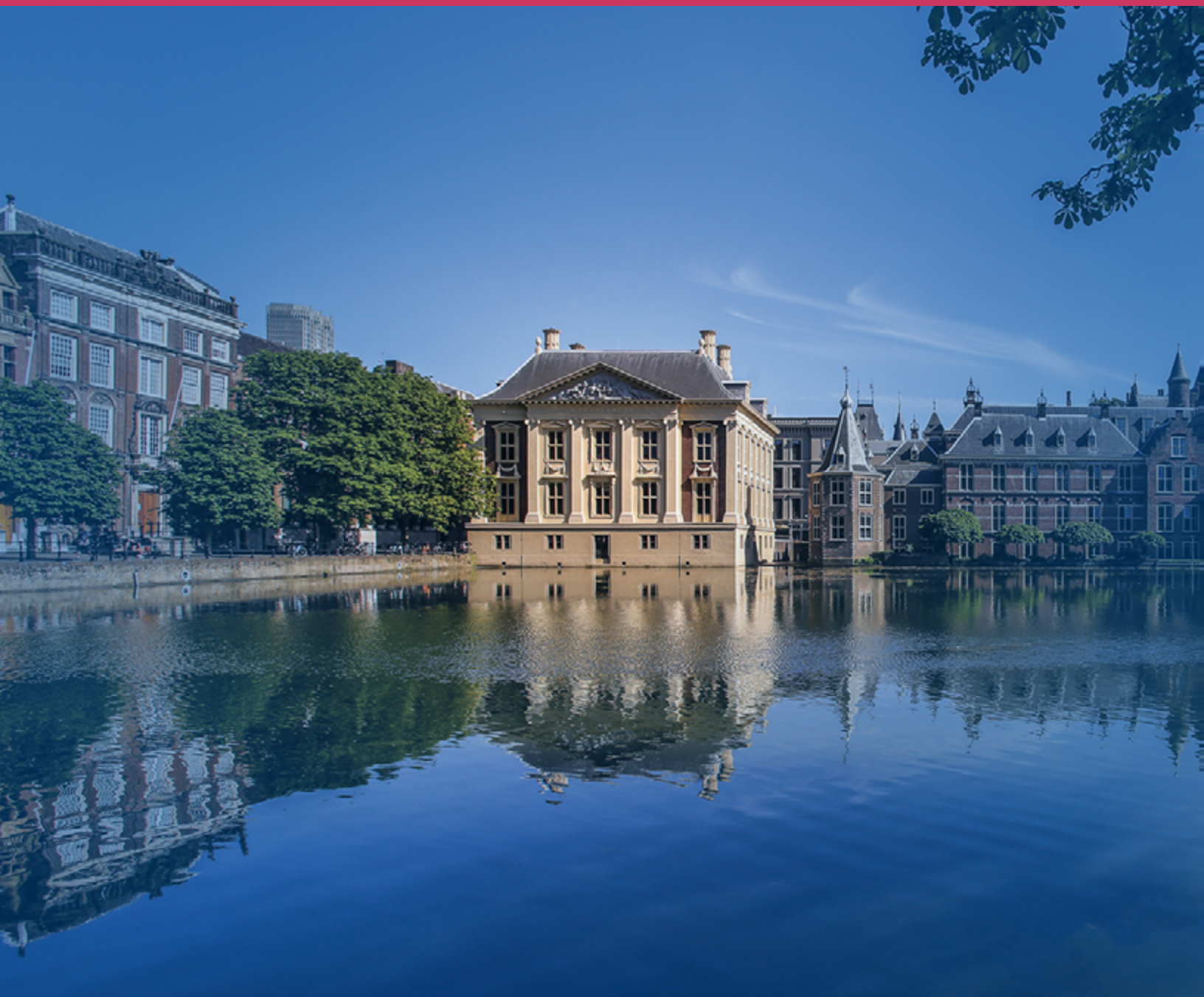
METABOLOMICS SOCIETY

15th Annual Conference of the Metabolomics Society

METABOLOMICS 2019

JUNE 23–27 | THE HAGUE

SCHEDULE OF ORAL PRESENTATIONS



AGENDA AT A GLANCE

Biomedical | Plant, Food, Environmental and Microbial | Technology | New Frontiers

SUNDAY, JUNE 23

	Atlantic	Alexia	Ariane	Oceania Foyer
11:00 a.m.	REGISTRATION OPEN			
12:30 p.m. – 2:15 p.m.	**W1:** EMN – Data Fusion	**W2:** Mining the Metabolome	**W3:** Multi-Omics Integration & Systems Metabolomics	**Intro to the Field 1:** Data Acquisition
2:30 p.m. – 4:15 p.m.	**W4:** Application of Graphical Models to Metabolomics	**W5:** Plant Metabolomes: Natural & Generated Variability	**W6:** How to Link Metabolome & Genome Mining	**Intro to the Field 1:** Data Acquisition
4:30 p.m. – 6:15 p.m.	**W7:** EMN – Professional Career Development	**W8:** Putting Metabolomic Data into Context	**W9:** An Open-Source Pipeline for Appraisal of NMR Datasets	**Intro to the Field 1:** Data Acquisition
6:30 p.m. – 8:30 p.m.	**Career Night** – Pacific			

MONDAY, JUNE 24

	Atlantic	Alexia	Ariane	Oceania Foyer
7:30 a.m.	REGISTRATION / INFO DESK OPEN			
8:30 a.m. – 10:15 a.m.	**W10:** The Importance of Quality Assurance & Quality Control	**W11:** Towards FAIR Spectral Libraries	**W12:** EMN – Stable Isotope-Resolved Metabolomics	**Intro to the Field 2:** Data (pre) Processing and Biostatistics
10:30 a.m. – 12:15 p.m.	**W13:** Beyond pathway mapping	**W14:** Standardizing the Fluxomics Workflows	**W15:** Tools to Study the Microbiome-Metabolome Interplay	**Intro to the Field 2:** Data (pre) Processing and Biostatistics
12:15 p.m. – 1:30 p.m.	LUNCH BREAK – ON YOUR OWN			
1:30 p.m. – 3:15 p.m.	**W16:** Application Metabolomics in Industry	**W17:** Dynamic Modeling of Human Metabolism	**W18:** EMN – Volatomics in Human Health	**Intro to the Field 2:** Data (pre) Processing and Biostatistics
3:30 p.m. – 5:00 p.m.	**Opening Ceremony** | **Plenary Session 1** – Joshua Rabinowitz – King Willem-Alexander Hall			
5:15 p.m. – 6:45 p.m.	**Welcome Reception – Poster Session 1** – Odd Numbers – Exhibit Foyer			
7:00 p.m. – 8:00 p.m.	**Metabolomics Society Town Hall Meeting –** Atlantic			

TUESDAY, JUNE 25

	Atlantic	King Willem-Alexander	Alexia	Ariane
7:45 a.m.	REGISTRATION / INFO DESK OPEN			
8:30 a.m. – 9:30 a.m.	**Plenary Session 2** – Dorret Boomsma – King Willem-Alexander Hall			
9:30 a.m. – 10:15 a.m.	BREAK – EXHIBIT FOYER			
10:15 a.m. – 12:00 p.m.	**1.** Cancer	**2.** Plant Applications 1	**3.** Data Integration & Data Basing 1	**4.** Novel Technologies
12:00 p.m. – 1:30 p.m.	LUNCH – IN FOYER WITH EXHIBITS – PLATINUM SPONSOR PRESENTATIONS			
12:20 p.m. – 1:20 p.m.			**Sponsor Pres:** SCIEX	**Sponsor Pres:** Waters Corporation
1:30 p.m. – 3:15 p.m.	**5.** Metabolic Disease	**6.** Food Applications 1	**7.** Flux Studies	**8.** Novel Instruments, Tools and Services
3:15 p.m. – 3:45 p.m.	BREAK – EXHIBIT FOYER			
3:45 p.m. – 5:30 p.m.	**9.** Epidemiology	**10.** Microbial Applications	**11.** Metabolite Identification 1	**12.** Stem Cells, Organoids
5:30 p.m. – 7:00 p.m.	**Poster Session 2** – Odd Numbers – Exhibit Foyer			
7:00 p.m. – 8:30 p.m.	**EMN Reception** – Pacific			

WEDNESDAY, JUNE 26

	Atlantic	King Willem-Alexander	Alexia	Ariane
8:00 a.m.	REGISTRATION / INFO DESK OPEN			
8:30 a.m. – 9:30 a.m.	**Plenary Session 3** – Cathie Martin – King Willem-Alexander Hall			
9:30 a.m. – 10:15 a.m.	BREAK – EXHIBIT FOYER			
10:15 a.m. – 12:00 p.m.	**13.** Lipidomics and Cardiovascular Disease	**14.** Plant Defense	**15.** Data Analysis & Statistics	**16.** Single Cell
12:00 p.m. – 1:30 p.m.	LUNCH – IN FOYER WITH EXHIBITS – PLATINUM SPONSOR PRESENTATIONS			
12:20 p.m. – 1:20 p.m.			**Sponsor Pres:** Thermo Fisher Scientific	**Sponsor Pres:** Shimadzu Europa GmbH
1:30 p.m. – 3:15 p.m.	**17.** Ageing and Disease	**18.** Food Applications 2	**19.** Data Integration & Data Basing 2	**20.** Regulatory Session
3:15 p.m. – 3:45 p.m.	BREAK – EXHIBIT FOYER			
3:45 p.m. – 5:30 p.m.	**21.** Infection and Immunity	**22.** Environment & Toxicology	**23.** New Instrumentation	**24.** Novel Applications
5:30 p.m. – 7:00 p.m.	**Poster Session 3** – Even Numbers – Exhibit Foyer			
7:30 p.m. – 10:30 p.m.	**Conference Dinner – Xiringuito**			

THURSDAY, JUNE 27

	Atlantic	King Willem-Alexander	Alexia	Ariane
8:30 a.m.	REGISTRATION / INFO DESK OPEN			
8:45 a.m. – 10:00 a.m.	**25.** Respiratory Diseases		**26.** Model Organisms	**27.** Genome-scale Modeling
10:00 a.m. – 10:45 a.m.	**Poster Session 4** – Even Numbers – Exhibit Foyer			
10:45 a.m. – 12:00 p.m.	**28.** Microbiome		**29.** Plant Applications 2	**30.** Metabolite Identification 2
12:00 p.m. – 1:30 p.m.	LUNCH – IN FOYER WITH EXHIBITS – PLATINUM SPONSOR PRESENTATIONS			
12:20 p.m. – 1:20 p.m			**Sponsor Pres:** Bruker Daltonics/Bruker Biospin	**Sponsor Pres:** Agilent Technologies
1:30 p.m. – 3:30 p.m	**Plenary Session 4** – Jean-Charles Portais – **Closing Ceremony** – King Willem-Alexander Hall			

BIOMEDICAL
PLANT, FOOD, ENVIRONMENTAL AND MICROBIAL

***AWARD WINNERS**

Monday, June 24		
Time	**Session**	**Location**
3:30 p.m. – 5:00 p.m.	**Opening Ceremony and Plenary Session 1** *Joshua Rabinowitz, Lewis-Sigler Institute, United States*	

Tuesday, June 25		
Time	**Session**	**Location**
8:30 a.m.– 9:30 a.m.	**Plenary Session 2** *Dorret I. Boomsma, Netherlands Twin Register, Vrije Universiteit, Netherlands*	
10:15 a.m. – 12:00 p.m.	**Session 1:** Cancer *(Session Chairs: Hunter Moseley & Maria Eugenia Monge)*	
10:15 a.m. – 10:45 a.m.	**1A SESSION KEYNOTE** Metabolomics Applications for Oncology and Immunology in Drug Discovery *Thomas Roddy, Agios Pharmaceuticals, United States*	Atlantic
10:45 a.m. – 11:05 a.m.	**1B** Multi-omic discovery of metabolic rewiring in triple-negative breast cancer following mitochondrial folate transport ablation *Steven Gross, Weill Cornell Medicine, United States*	
11:05 a.m. – 11:20 a.m.	**1C** Investigating the metabolic response of cancer cells to indisulam *Lili Herendi, PhD student, United Kingdom*	
11:20 a.m. – 11:40 a.m.	**1D** Rewiring of energy metabolism drives resistance to the proteasome inhibitor bortezomib *Esther Zaal, Biomolecular Mass Spectrometry and Proteomics, Utrecht University, Netherlands*	
11:40 a.m. – 11:55 a.m.	**1E*** Understanding metabolite heterogeneity in pancreatic ductal adenocarcinoma, and the role of adaptive metabolic reprogramming in chemotherapy resistance *Sarah Hancock, University of New South Wales, Australia*	
10:15 a.m. – 12:00 p.m.	**Session 2:** Plant Applications 1 *(Session Chairs: Sanjay Swarup & Jasen Finch)*	
10:15 a.m. – 10:45 a.m.	**2A SESSION KEYNOTE** The volatile flavor composition network in tomato and its modification *Antonio Granell, CSIC, Spain*	King Willem Alexander
10:45 a.m. – 11:05 a.m.	**2B** Developing Advanced and Integrated Metabolomics Technologies to Address the Grand Challenges of Metabolite Identification and Depth of Coverage *Lloyd Sumner, University of Missouri, United States*	
11:05 a.m. – 11:20 a.m.	**2C*** From MS peak to unambiguous metabolite identification using the WeizMass spectral library and LC-MS-SPE-NMR system *Adam Jozwiak, Weizmann Institute of Science, Israel*	
11:20 a.m. – 11:40 a.m.	**2D** Chocolate metabolomics *Robert Hall, Wageningen UR, Netherlands*	
11:40 a.m. – 11:55 a.m.	**2E** A tissue specific metabolomic study in hybrid aspen *Ilara Budzinski, Swedish University of Agricultural Sciences (SLU), Sweden*	

TECHNOLOGY
NEW FRONTIERS

*AWARD WINNERS

Tuesday, June 25		
Time	**Session**	**Location**
10:15 a.m. – 12:00 p.m.	**Session 3:** Data Integration & Data Basing 1 *(Session Chairs: Fabien Jourdan & Natasa Giallourou)*	
10:15 a.m. – 10:45 a.m.	**3A SESSION KEYNOTE** The Internet for Social Machines *Barend Mons, GO FAIR, Netherlands*	Princess Alexia
10:45 a.m. – 11:05 a.m.	**3B** Matching Untargeted Liquid Chromatography - Mass Spectrometry Features Across Multiple Cohorts: Finding the Same Needles in Several Haystacks Via Networks *Rui Climaco Pinto, Imperial College London, United Kingdom*	
11:05 a.m. – 11:20 a.m.	**3C*** Visualizing metabolomics data in directed biological networks *Denise Slenter, Maastricht University, Netherlands*	
11:20 a.m. – 11:40 a.m.	**3D** High-throughput metabolomics identifies substrate-enzyme relationships in a metabolism-wide CRISPR interference library *Hannes Link, Max Planck Institute for Terrestrial Microbiology, Germany*	
11:40 a.m. – 11:55 a.m.	**3E*** Weighting strategies for the analysis of secondary outcomes in nested case-control metabolomics data *Gerard Gonzales, Ghent University, Belgium*	
10:15 a.m. – 12:00 p.m.	**Session 4:** Novel Technologies *(Session Chairs: Rob Vreeken & Lieven van Meulebroek)*	
10:15 a.m. – 10:45 a.m.	**4A SESSION KEYNOTE** Improving Technologies for High Throughput and Miniaturized Metabolomics for Precision Medicine *Thomas Hankemeier, Leiden University, Netherlands*	Princess Ariane
10:45 a.m. – 11:05 a.m.	**4B** Investigation of host-microbiota co-metabolism as a new strategy for biomarker discovery – New Chemical Biology tools for Metabolomics analysis *Daniel Globisch, Uppsala University, Sweden*	
11:05 a.m. – 11:20 a.m.	**4C*** GC×GC-TOFMS and SIFT-MS approaches for clinical breath-based asthma phenotyping *Pierre-Hugues Stefanuto, Liège University, Belgium*	
11:20 a.m. – 11:40 a.m.	**4D** Mathematical modelling of metabolism: a driver for developing personalized and precision medicine *Natal van Riel, Eindhoven University of Technology, Netherlands*	
11:40 a.m. – 11:55 a.m.	**4E** TIMS and PASEF multiply speed and sensitivity in lipidomics *Catherine G. Vasilopoulou, Max Planck Institute of Biochemistry, Germany*	

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PLANT, FOOD, ENVIRONMENTAL AND MICROBIAL

***AWARD WINNERS**

Tuesday, June 25		
Time	**Session**	**Location**
1:30 p.m. – 3:15 p.m.	**Session 5:** Metabolic Disease *(Session Chairs: Christophe Junot & Katharina Herzog)*	
1:30 p.m. – 2:00 p.m.	**5A SESSION KEYNOTE** Integrating epidemiologic, pharmacologic, genetic and gut microbiome data in the BBMRI-NL drug-metabolome atlas *Cornelia van Duijn, University of Oxford, United Kingdom*	Atlantic
2:00 p.m. – 2:20 p.m.	**5B** Metabolic profiling of tissue-specific insulin resistance in human obesity: Results from the Diogenes Study and The Maastricht Study *Ilja Arts, Epidemiology & MaCSBio, Maastricht University, Netherlands*	
2:20 p.m. – 2:35 p.m.	**5C** Identification of novel metabolites in alkaptonuria by LC-QTOF-MS profiling and flux analysis of a targeted HGD-/- mouse model *Brendan Norman, Institute of Ageing & Chronic Disease, University of Liverpool, United Kingdom*	
2:35 p.m. – 2:55 p.m.	**5D*** Combining untargeted metabolomics, human genetics, causal inference, and pathway enrichment to define the obesity metabolome *Yu-Han Hsu, Harvard Medical School, United States*	
2:55 p.m. – 3:10 p.m.	**5E*** Metabolomics of Ndufs4-/- skeletal muscle: adaptive mechanisms converge at the ubiquinone-cycle *Karin Terburgh, North-West University, South Africa*	
1:30 p.m. – 3:15 p.m.	**Session 6:** Food Applications 1 *(Session Chairs: Cristina Andres Lacueva & Jessica Cooperstone)*	
1:30 p.m. – 2:00 p.m.	**6A SESSION KEYNOTE** A metabolomic study on coffee – From coffee brews to liver cancer risk *Augustin Scalbert, International Agency for Research on Cancer (IARC), France*	King Willem Alexander
2:00 p.m. – 2:20 p.m.	**6B** Integrated analysis of metabolomics and microbiome data showing additional dietary effects *Jildau Bouwman, TNO, Netherlands*	
2:20 p.m. – 2:35 p.m.	**6C** Quantitative Dietary Fingerprinting (QDF)—A Novel Tool for Comprehensive Dietary Assessment Based on Urinary Nutrimetabolomics *Raúl González-Domínguez, Biomarkers and Nutrimetabolomics Laboratory, University of Barcelona, Spain*	
2:35 p.m. – 2:55 p.m.	**6D** Grass, beef and human. Unlocking the value of the food chain in New Zealand *Arvind Subbaraj, AgResearch Ltd., New Zealand*	
2:55 p.m. – 3:10 p.m.	**6E** NMR metabolomics revealed different impact of non-acylated and acylated anthocyanins on plasma metabolic profiles in obese diabetic Zucker rats *Kang Chen, University of Turku, Finland*	

TECHNOLOGY
NEW FRONTIERS

***AWARD WINNERS**

Tuesday, June 25		
Time	**Session**	**Location**
1:30 p.m. – 3:15 p.m.	**Session 7:** Flux Studies *(Session Chairs: Barbara Bakker & Bekzod Khakimov)*	
1:30 p.m. – 2:00 p.m.	**7A SESSION KEYNOTE** A systems medicine approach to identify new drug targets: Model-driven discovery of metabolic reprogramming in metastatic prostate cancer *Marta Cascante, University of Barcelona, Spain*	Princess Alexia
2:00 p.m. – 2:20 p.m.	**7B** Using stable-isotope labelled metabolomics to explore cell-cell communication between malaria parasites and host cells *Darren Creek, Monash University, Australia*	
2:20 p.m. – 2:35 p.m.	**7C*** Using deuterium labelled glucose to quantify redox metabolism in plants *Edward Smith, University of Oxford, United Kingdom*	
2:35 p.m. – 2:55 p.m.	**7D*** Modelling Cancer Lipogenesis using REIMS Metabolic Flux analysis in breast cancer cell lines *Seyma Turkseven, Imperial College London, United Kingdom*	
2:55 p.m. – 3:10 p.m.	**7E*** Exploring the use of GC-CI-MS for stable isotope labeling in metabolomics *Jordi Capellades Tomàs, IISPV, Spain*	
1:30 p.m. – 3:15 p.m.	**Session 8:** Novel Instrumentations, Tools and Services *(Presented by Platinum and Gold Sponsors)* *(Session Chairs: Thomas Hankemeier & David Wishart)*	
1:30 p.m. – 2:30 p.m.	**PLATINUM PRESENTERS AND PANEL DISCUSSION** **Agilent Technologies:** Christine Miller, Omics Market Manager, USA **Bruker Daltonics/Bruker BioSpin:** Lucy Woods, phD, Product Manager QTOF, Germany **SCIEX:** Baljit Ubhi, Market Manager - Metabolomics Business, USA **Shimadzu:** Emily Armitage, Research Scientist, UK **Thermo Fisher Scientific:** Amanda Souza, Manager, Product Marketing, USA **Waters Corporation:** David Heywood, Senior Manager Omics Business Development, UK	Princess Ariane
2:30 p.m. – 3:15 p.m	**GOLD PRESENTERS AND PANEL DISCUSSION** **Biocrates Life Sciences AG:** Therese Koal, PhD, Head of Research & Development, Austria **Cambridge Isotope Laboratories, Inc:** Krista Backiel, Marketing and Metabolomics Manager, USA **Human Metabolome Technologies:** Tom Hoshiba, Managing Director, Netherlands **Metabolon:** Alex Forrest-Hay, VP Population Health, USA	

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***AWARD WINNERS**

Tuesday, June 25		
Time	**Session**	**Location**
3:45 p.m. – 5:30 p.m.	**Session 9:** Epidemiology *(Session Chairs: Krista Zanetti & Julie Schmidt)*	
3:45 p.m. – 4:15 p.m.	**9A SESSION KEYNOTE** Integrating metabolomics with genomics, proteomics, and other omics for health and drug research *Karsten Suhre, Weill Cornell Medicine - Qatar, Qatar*	Atlantic
4:15 p.m. – 4:35 p.m.	**9B** Application of 1H NMR metabolomics in ~7,000 people to investigate potential molecular mechanisms of genetic risk variants for coronary artery diseases *Ibrahim Karaman, Imperial College London, United Kingdom*	
4:35 p.m. – 4:50 p.m.	**9C** Untargeted metabolomics in a prospective cohort to identify diet-related metabolites associated with age-related cognitive decline *Dorrain Low, Lee Kong Chian School of Medicine, Nanyang Technological University, Singapore*	
4:50 p.m. – 5:10 p.m.	**9D** Metabolic profile and the risk of developing prostate cancer - A nested-case control study *Ali Moazzami, Department of Molecular Sciences, SLU, Sweden*	
5:10 p.m. – 5:25 p.m.	**9E** The Metabolome of BMI: A COnsortium of METabolomics Studies (COMETS) Meta-analysis of 85,000 adults *Rachel Kelly, HMS and BWH, United States*	
3:45 p.m. – 5:30 p.m.	**Session 10:** Microbial Applications *(Session Chairs: Adriana Carvalho de Souza & Douglas McCloskey)*	
3:45 p.m. – 4:15 p.m.	**10A SESSION KEYNOTE** Functional characterization of Escherichia coli lipid genes *Jos Brouwers, Utrecht University, Netherlands*	King Willem Alexander
4:15 p.m. – 4:35 p.m.	**10B** Metabolomics-based engineering biology of microorganisms *Tomohisa Hasunuma, Engineering Biology Research Center, Kobe University, Japan*	
4:35 p.m. – 4:50 p.m.	**10C*** Expanding the Applications of Rapid Evaporative Ionisation Mass Spectrometry (REIMS) to the Pharmaceutical Product Development Workflow *Toma Ramonaite, Imperial College London, United Kingdom*	
4:50 p.m. – 5:10 p.m.	**10D** Linking metabolic function to member taxa in complex microbial communities using metabolome-guided multi-omics *Nay Min Min Thaw Saw, Singapore Center for Environmental Life Science Engineering, Singapore*	
5:10 p.m. – 5:25 p.m.	**10E*** Microbial metabolic networks: the hidden key to resilience of coral algal endosymbionts *Jennifer Matthews, University of Technology Sydney, Australia*	

TECHNOLOGY
NEW FRONTIERS

*AWARD WINNERS

Tuesday, June 25		
Time	**Session**	**Location**
3:45 p.m. – 5:30 p.m.	**Session 11:** Metabolite Identification 1 *(Session Chairs: Justin van der Hooft & Sonia Liggi)*	
3:45 p.m. – 4:15 p.m.	**11A SESSION KEYNOTE** Infrared ion spectroscopy: new opportunities for molecular structure identification in MS-based metabolomics *Jos Oomens, Radboud University, Netherlands*	Princess Alexia
4:15 p.m. – 4:35 p.m.	**11B** mFam – prediction of metabolite families based on spectral data *Hendrik Treutler, Dept. of Biochemistry of Plant Interactions, Leibniz Institute of Plant Biochemistry, Germany*	
4:35 p.m. – 4:50 p.m.	**11C*** Supercharging Comparative Metabolomics with METABOseek *Maximilian Helf, Cornell University / Boyce Thompson Institute, United States*	
4:50 p.m. – 5:10 p.m.	**11D** Ion mobility – mass spectrometry based multi-dimensional metabolite annotation *Zhiwei Zhou, IRCBC, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, China*	
5:10 p.m. – 5:25 p.m.	**11E*** Recommending substructures for unknown tandem mass spectra *Youzhong LIU, University of Antwerp, Belgium*	
3:45 p.m. – 5:30 p.m.	**Session 12:** Stem Cells/Organoids/Organ-on-a-Chip *(Session Chairs: Alain van Gool & Isabelle Kohler)*	
3:45 p.m. – 4:15 p.m.	**12A SESSION KEYNOTE** No transporters means no transport – and assessment of the 'real' (natural) substrates of xenobiotic transporters *Douglas Kell, University of Liverpool, United Kingdom*	Princess Ariane
4:15 p.m. – 4:35 p.m.	**12B** Spatial Isotope tracer Metabolomics to study 13C labelled Metabolite Distribution in 3D Tumor Spheroid Cell culture *Prasad Phapale, EMBL, Germany*	
4:35 p.m. – 4:50 p.m.	**12C*** Microengineered Human Blood Vessel for Next Generation Drug Discovery *Abidemi Junaid, Systems Biomedicine and Pharmacology, LACDR, Leiden University, Netherlands*	
4:50 p.m. – 5:10 p.m.	**12D*** Stable Isotope-Resolved Metabolomics (SIRM) Defines DEK Oncogene Driven Metabolic Reprogramming in 3D Epidermal Organoids *Sara Vicente-Muñoz, NMR-Based Metabolomics Core Facility, Division of Pathology and Laboratory Medicine, United States*	
5:10 p.m. – 5:25 p.m.	**12E** Metabolomics as a quality control for the production of chondrogenic microtissues towards characterized endochondral bone regeneration *Niki Loverdou, Prometheus, Division of Skeletal Tissue Engineering, KULeuven, Belgium*	

BIOMEDICAL
PLANT, FOOD, ENVIRONMENTAL AND MICROBIAL

Wednesday, June 26		
Time	**Session**	**Location**
8:30 a.m. – 9:30 a.m.	**Plenary Session 2** *Cathie Martin, John Innes Centre, Colney Research Park, UK*	
10:15 a.m. – 12:00 p.m.	**Session 13:** Lipidomics and Cardiovascular Disease *(Session Chairs: Jules Griffin & Aline Martins)*	
10:15 a.m. – 10:45 a.m.	**13A SESSION KEYNOTE** High-throughput lipidomic quantitation of human blood in cancer screening *Michal Holcapek, University of Pardubice, Czech Republic*	Atlantic
10:45 a.m. – 11:05 a.m.	**13B** Changes in plasma lipids predict pravastatin efficacy in secondary prevention *Peter Meikle, Baker Heart and Diabetes Institute, Australia*	
11:05 a.m. – 11:20 a.m.	**13C*** Metabolomics analysis of human atherosclerotic plaques reveals a potential novel pathway of macrophage foam cell apoptosis in advanced atherosclerosis *Panagiotis Vorkas, Imperial College London, United Kingdom*	
11:20 a.m. – 11:40 a.m.	**13D** Plasma metabolomics profiles associated with endothelial health and dysfunction impose changes to endothelial glycan biosynthesis and reflect endothelial catecholamine response *Óttar Rolfsson, University of Iceland, Iceland*	
11:40 a.m. – 11:55 a.m.	**13E** Sphingolipidomics investigation of the ischemic brain injury *Ching-Hua Kuo, National Taiwan University, Taiwan*	
10:15 a.m. – 12:00 p.m.	**Session 14:** Plant Defense *(Session Chairs: Annick Moing & Halford Dace)*	
10:15 a.m. – 10:45 a.m.	**14A SESSION KEYNOTE** Elucidating insect resistance in tomato through genetical metabolomics *Ric de Vos, Bioscience, Wageningen Plant Research, Wageningen University and Research, Netherlands*	King Willem Alexander
10:45 a.m. – 11:05 a.m.	**14B** Dissecting the Genetic Basis of Variation in Tomato Fruit Metabolism and Pathogen Resistance through Multimodal Investigation of Wild Species Introgressions *Jedrzej Szymanski, Leibniz Institute of Plant Genetics and Crop Plant Research, Germany*	
11:05 a.m. – 11:20 a.m.	**14C** Metabolomics application to unravel the biochemistry underlying enhancement of drought stress tolerance in crops by plant growth promoting rhizobacteria *Fidele Tugizimana, University of Johannesburg, South Africa*	
11:20 a.m. – 11:40 a.m.	**14D** A strategy for the discovery and characterisation of health and decline biomarkers in British Oak trees using non-targeted metabolomics *Jasen Finch, Aberystwyth University, United Kingdom*	
11:40 a.m. – 11:55 a.m.	**14E*** Linking the volatilome and metabolome via plant defenses: stimulation of the salicylic acid pathway recruits natural enemies below ground *Camila Filgueiras, Cornell University, United States*	

TECHNOLOGY
NEW FRONTIERS

*AWARD WINNERS

Wednesday, June 26		
Time	**Session**	**Location**
10:15 a.m. – 12:00 p.m.	**Session 15:** Data Analysis & Statistics *(Session Chairs: Age Smilde & Isabel Orf)*	
10:15 a.m. – 10:45 a.m.	**15A SESSION KEYNOTE** Is Metabolomics ready for the return of Artificial Neural Networks? *David Broadhurst, Edith Cowan University, Australia*	Princess Alexia
10:45 a.m. – 11:05 a.m.	**15B** MS-DIAL 4.0: a computational workflow for ion mobility tandem mass spectrometry data in metabolomics *Hiroshi Tsugawa, RIKEN, Japan*	
11:05 a.m. – 11:20 a.m.	**15C*** Chemically informed distance metrics for tandem mass spectrometry data *Madeleine Ernst, Department of Congenital Disorders, Statens Serum Institut, Denmark*	
11:20 a.m. – 11:40 a.m.	**15D** Identifying biologically relevant modules in metabolomics and lipidomics data with Differential Network-based Enrichment Analysis (DNEA) *Alla Karnovsky, University of Michigan, United States*	
11:40 a.m. – 11:55 a.m.	**15E** Signature Mapping (SigMa): A new automatic tool for rapid processing of complex urine NMR spectra *Bekzod Khakimov, University of Copenhagen, Denmark*	
10:15 a.m. – 12:00 p.m.	**Session 16:** Single Cell *(Session Chairs: Jildau Bouwman & Michel van Weeghel)*	
10:15 a.m. – 10:45 a.m.	**16A SESSION KEYNOTE** Spatial metabolomics in tissues and single cells *Theodore Alexandrov, EMBL, Germany*	Princess Ariane
10:45 a.m. – 11:05 a.m.	**16B** Comprehensive Single Cell Multi Omics *Christian Berchtold, Institute for Chemistry and Bioanalytics, Switzerland*	
11:05 a.m. – 11:20 a.m.	**16C** Quantifying heterogeneity in drug uptake, metabolism and effect using Raman spectroscopy and mass spectrometry on the single-cell level *Ahmed Ali, Leiden University, The Netherlands | RIKEN, Japan, Japan*	
11:20 a.m. – 11:40 a.m.	**16D*** Relationships between cellular metabolite and drug uptake and transporter expression profiles *Marina Muelas, University of Liverpool, United Kingdom*	
11:40 a.m. – 11:55 a.m.	**16E*** A Single-Cell Look at Biological Nitrogen Fixation: Direct Determination of Metabolite Formulas from Isotopic Fine Structures in Heterogeneous Cell Populations *Tina Tran, The George Washington University, United States*	

BIOMEDICAL
PLANT, FOOD, ENVIRONMENTAL AND MICROBIAL

***AWARD WINNERS**

Wednesday, June 26		
Time	**Session**	**Location**
1:30 p.m. – 3:15 p.m.	**Session 17:** Ageing and Disease *(Session Chairs: Matej Oresic & Candice Ulmer)*	
1:30 p.m. – 2:00 p.m.	**17A SESSION KEYNOTE** Multiomic data integration using machine learning and data-driven inverse metabolic modelling - from diabetes to immune system modulation *Wolfram Weckwerth, University of Vienna, Austria*	Atlantic
2:00 p.m. – 2:20 p.m.	**17B** Mass spectrometric analysis of sebum contents for classification of Parkinson's disease *Drupad Trivedi, University of Manchester, United Kingdom*	
2:20 p.m. – 2:35 p.m.	**17C** Mechanistic model-driven exometabolomic characterisation of human dopaminergic neuronal metabolism *Ronan Fleming, Leiden University, Netherlands*	
2:35 p.m. – 2:55 p.m.	**17D** Interleaving metabolic effects of sleep and aging *Arjun Sengupta, University of Pennsylvania, United States*	
2:55 p.m. – 3:10 p.m.	**17E** Analysis of changes in the eye lens and aqueous humor under cataract development using quantitative metabolomics *Vadim Yanshole, ITC SB RAS / NSU, Russian Federation*	
1:30 p.m. – 3:15 p.m.	**Session 18:** Food Applications 2 *(Session Chairs: Sastia Putri & Johanna Jokioja)*	
1:30 p.m. – 2:00 p.m.	**18A SESSION KEYNOTE** Rapid Evaporative Ionisation Mass Spectrometry for detecting compounds related to consumer liking of meat *Alastair Ross, AgResearch, New Zealand*	King Willem Alexander
2:00 p.m. – 2:20 p.m.	**18B** Fiber mix supplementation in wheat-based flatbreads delays the exogenous appearance of glucose and its downstream metabolites *Lisa Schlicker, BRICS, TU Braunschweig, Germany*	
2:20 p.m. – 2:35 p.m.	**18C*** A metabolomic approach to the identification and validation of biomarkers of apple intake *Aoife McNamara, Institute of Food and Health, Ireland*	
2:35 p.m. – 2:55 p.m.	**18D** Brainfood metabolomics study (Icebreaker, Brave sub-study) *Kati Hanhineva, Afekta Technologies Ltd., Finland*	
2:55 p.m. – 3:10 p.m.	**18E*** Mass spectrometry based non-targeted metabolomics enables the identification of Amadori products in feces of formula-fed infants *Alesia Walker, Helmholtz Zentrum München, Research Unit Analytical BioGeochemistry, Germany*	

Wednesday, June 26		
Time	**Session**	**Location**
1:30 p.m. – 3:15 p.m.	**Session 19:** Data Integration & Data Basing 2 *(Session Chairs: Dan Raftery & Dara Daygon)*	
1:30 p.m. – 2:00 p.m.	**19A SESSION KEYNOTE** The UniProt, Rhea, and SwissLipids knowledge resources for metabolomics and lipidomics *Alan Bridge, Swiss-Prot group, SIB Swiss Institute of Bioinformatics, Switzerland*	Princess Alexia
2:00 p.m. – 2:20 p.m.	**19B** RIKEN Plant Metabolome MetaDatabase: an integrated plant metabolome data repository based on the semantic web *Atsushi Fukushima, RIKEN Center for Sustainable Resource Science, Japan*	
2:20 p.m. – 2:35 p.m.	**19C** Contextualizing Metabolomics Data by Integrating Text Mining and Machine Learning *Magnus Palmblad, Leiden University Medical Center, Netherlands*	
2:35 p.m. – 2:55 p.m.	**19D** Metabolic Reaction Network-based Recursive Metabolite Annotation for Untargeted Metabolomics *Zheng-Jiang Zhu, Chinese Academy of Sciences (CAS), China*	
2:55 p.m. – 3:10 p.m.	**19E** Sparse Multi-block PLS for Selection of Related Signals in Multi-platform Metabolomics Data *Timothy Ebbels, Imperial College London, United Kingdom*	
1:30 p.m. – 3:15 p.m.	**Session 20:** Regulatory Session Translating metabolomics from academic science into regulatory practice: challenges and progress in pharmacology and toxicology *(Session Chair: Pim Leonards)*	
1:30 p.m. – 1:50 p.m.	An Overview of the 21st Century Cures Act: Opportunities for Biomarkers and Precision Medicine *Dr. Rick Beger, National Center for Toxicological Research, US FDA, United States*	Princess Ariane
1:50 p.m. – 2:10 p.m.	Big Data "Omics" – Challenges and Opportunities in Regulation *Dr. Renate König, Paul-Ehrlich-Institut, Federal Institute for Vaccines and Biomedicines, Germany*	
2:10 p.m. – 2:30 p.m.	Various Applications of Metabolomics in Toxicology *Prof Hennicke Kamp, BASF, Germany*	
2:30 p.m. – 2:50 p.m.	Best Practice Guidelines and Reporting Standards for Applications of Metabolomics in Regulatory Toxicology: the International MERIT Project *Prof. Mark Viant, University of Birmingham, UK*	
2:50 p.m. – 3:15 p.m.	Panel Discussion with all presenters, moderated by Pim Leonards	

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Wednesday, June 26		
Time	**Session**	**Location**
3:45 p.m. – 5:30 p.m.	**Session 21:** Infection and Immunity *(Session Chairs: Darren Creek & Xinzhu Wang)*	
3:45 p.m. – 4:15 p.m.	**21A SESSION KEYNOTE** Understanding the metabolic perturbation in severe fever with thrombocytopenia syndrome *Zeping Hu, Tsinghua University, China*	Atlantic
4:15 p.m. – 4:35 p.m.	**21B** Hijacking of host cellular function by opportunistic pathogens during intracellular infections *Volker Behrends, University of Roehampton, United Kingdom*	
4:35 p.m. – 4:50 p.m.	**21C*** Diagnosis of Aspergillosis based on metabolomics data – application of relative expression analysis-RXA to minimize interindividual metabolic differences *Joanna Godzien, Medical University of Bialystok, Clinical Research Centre, Poland*	
4:50 p.m. – 5:10 p.m.	**21D** Alterations of systematic metabolism upon viral infection: from metabolite profiling to isotope tracing. *Kristaps Klavins, CeMM - Research Center for Molecular Medicine, Austria*	
5:10 p.m. – 5:25 p.m.	**21E*** Characterisation of the human milk lipidome using liquid chromatography-ion mobility spectroscopy-mass spectrometry reveals novel lipids *Alexandra George, The University of Western Australia, School of Molecular Sciences, Australia*	
3:45 p.m. – 5:30 p.m.	**Session 22:** Environment & Toxicology *(Session Chairs: Melissa Fitzgerald and Ralf Weber)*	
3:45 p.m. – 4:15 p.m.	**22A SESSION KEYNOTE** Metabolomics and toxicity studies of zebrafish embryos exposed to environmental contaminants *Pim Leonards, Vrije Universiteit, Netherlands*	King Willem Alexander
4:15 p.m. – 4:35 p.m.	**22B** Gestational and post-natal exposure to ambient air pollution: a metabolomics approach *Marina Tavares, University of Sao Paulo, Brazil*	
4:35 p.m. – 4:50 p.m.	**22C** Association between coffee consumption, plasma metabolites and hypertension risk *Wei Jie Seow, National University of Singapore, Singapore*	
4:50 p.m. – 5:10 p.m.	**22D** Small molecules and lipids preserved over thousands of years in mummified humans *Kevin Quinn, University of Colorado Anschutz, United States*	
5:10 p.m. – 5:25 p.m.	**22E** Food preservative zinc oxide nanoparticles (ZnONPs) induces neurobehavioral deficits in mice with altered gut microbiome and dysregulated serum and hippocampus metabolome *Chang Chen, Chongqing Medical University, China*	

TECHNOLOGY
NEW FRONTIERS

*AWARD WINNERS

Wednesday, June 26		
Time	**Session**	**Location**
3:45 p.m. – 5:30 p.m.	**Session 23:** New Instrumentation *(Session Chairs: Rawi Ramautar & Charmion Cruickshank-Quinn)*	
3:45 p.m. – 4:15 p.m.	**23A SESSION KEYNOTE** Integration of MS imaging and LC-MS techniques – discovering tissue heterogeneity with the accuracy and depth of traditional profiling tools *Matthew Lewis, Imperial College London, United Kingdom*	Princess Alexia
4:15 p.m. – 4:35 p.m.	**23B** Mapping Hydrophilic Intermediates of the Central Carbon and Energy Metabolism (CCEM) by Ion Pairing and Ion Exchange Chromatography – Tandem MS *Gerd Balcke, Leibniz-Institute of Plant Biochemistry, Germany*	
4:35 p.m. – 4:50 p.m.	**23C*** High-Resolution µ-scaled Magic-Angle Spinning NMR Mapping of diseased rat brains *Covadonga Lucas-Torres, CEA Saclay, France*	
4:50 p.m. – 5:10 p.m.	**23D** Electroextraction-based sample preparation strategies for enrichment of low-abundant metabolites *Peter Lindenburg, Analytical Biosciences & Metabolomics, Leiden Centre for Applied Bioscience, Leiden University, Netherlands*	
5:10 p.m. – 5:25 p.m.	**23E** How to automate boring lipidomic extraction? *Justine Bertrand-Michel, MetaToul-Lipidomic, France*	
3:45 p.m. – 5:30 p.m.	**Session 24:** Novel Applications *(Session Chairs: Lorraine Brennan & Bert Wouters)*	
3:45 p.m. – 4:15 p.m.	**24A SESSION KEYNOTE** Metabolomics: Central Approach for Study of the Exposome *Dean Jones, Emory University, United States*	Princess Ariane
4:15 p.m. – 4:35 p.m.	**24B** Metabolomes of mitochondrial diseases and inclusion body myositis patients: treatment targets and biomarkers *Vidya Velagapudi, FIMM, University of Helsinki, Finland*	
4:35 p.m. – 4:50 p.m.	**24C** Boosting anti-doping screening through metabolomics *Luca Narduzzi, Oniris - Laberca, France*	
4:50 p.m. – 5:10 p.m.	**24D** A Novel Metabolomics Method for Quantitative Analysis of over 1,000 Metabolites *Guowang Xu, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China*	
5:10 p.m. – 5:25 p.m.	**24E** Post-mortem changes in the metabolomic profiles of animal and human tissues *Ekaterina Zelentsova, International Tomography Center SB RAS, Novosibirsk, Russia; Novosibirsk State University, Russian Federation*	

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TECHNOLOGY

*AWARD WINNERS

Thursday, June 27

Time	Session	Location
8:45 a.m. – 10:00 a.m.	**Session 25:** Respiratory Diseases *(Session Chairs: Nichole Reisdorph & Priyanka Choudhury)*	
8:45 a.m. – 9:15 a.m.	**25A SESSION KEYNOTE** Omega-6 polyunsaturated fatty acid metabolites are associated with vitamin D levels in early life *Jessica Lasky-Su, Brigham and Women's Hospital, United States*	Atlantic
9:15 a.m. – 9:40 a.m.	**25B** Comprehensive metabolomic and immulogical profiling of Asthma COPD Overlap (ACO) *Nilanjana Ghosh, School of Medical Science and Technology, India*	
9:40 a.m. – 9:55 a.m.	**25C*** The relationship between the maternal metabolome and childhood asthma: results from the Vitamin D Antenatal Asthma Reduction Trial (VDAART) *Mengna Huang, Channing Division of Network Medicine, Brigham and Women's Hospital and Harvard Medical School, United States*	
8:45 a.m. – 10:00 a.m.	**Session 26:** Model Organisms *(Session Chairs: Oliver Jones & Lyudmila Yanshole)*	
8:45 a.m. – 9:15 a.m.	**26A SESSION KEYNOTE** Can Stage-Specific Metabolites be Recovered from Mixed-Stage C. elegans Cultures? *Arthur Edison, University of Georgia, United States*	Princess Alexia
9:15 a.m. – 9:40 a.m.	**26B** Bringing together what belongs together – Bridging the Caenorhabditis elegans model organism database, genome scale model and metabolite databases *Michael Witting, Research Unit Analytical BioGeoChemistry, Helmholtz Zentrum München, Germany*	
9:40 a.m. – 9:55 a.m.	**26C*** The use of mitochondrial metabolomics in discovering the molecular function of a mitochondrial membrane protein *Daqiang Pan, Centre for Biological Systems Analysis, University of Freiburg, Germany*	
8:45 a.m. – 10:00 a.m.	**Session 27:** Genome-Scale Modeling *(Session Chairs: Gabi Kastenmüller & Patrick Trainor)*	
8:45 a.m. – 9:15 a.m.	**27A SESSION KEYNOTE** Computational modelling of host-microbiome co-metabolism *Ines Thiele, National University of Ireland, Ireland*	Princess Ariane
9:15 a.m. – 9:40 a.m.	**27B** Metabollic footprint of Parkinson's Disease: integration of patient-derived X-omics data with a human genome-scale model. *Agnieszka Wegrzyn, LACDR, Leiden University, Netherlands*	
9:40 a.m. – 9:55 a.m.	**27C** Genome-wide metabolic modeling of human CD4+ T-helper cells differentiation unraveled the relative importance of ceramides *Partho Sen, Postdoctoral Researcher, Finland*	

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TECHNOLOGY

***AWARD WINNERS**

Thursday, June 27		
Time	**Session**	**Location**
10:45 a.m. – 12:00 p.m.	**Session 28:** Microbiome *(Session Chairs: Guowang Xu & Madeleine Ernst)*	
10:45 a.m. – 11:15 a.m.	**28A SESSION KEYNOTE** Global Chemical Impacts of the Microbiome Include Novel Conjugated Bile Acids that Stimulate FXR *Robert Quinn, Michigan State University, United States*	Atlantic
11:15 a.m. – 11:40 a.m.	**28B*** Exploring the microbiota-host epigenetics axis in female and male germ-free and conventional mice *Joan Miró Blanch, Metabolomics Platform, IISPV & Department of Electronic Engineering, Universitat Rovira i Virgili, Spain*	
11:40 a.m. – 11:55 a.m.	**28C*** Individual Variations in Plasma Metabolites are Driven by Diet, Genetics and Gut Microbiome *Lianmin Chen, University Medical Centre Groningen, Netherlands*	
10:45 a.m. – 12:00 p.m.	**Session 29:** Plant Applications 2 *(Session Chairs: Lloyd Sumner & Adam Jozwiak)*	
10:45 a.m. – 11:15 a.m.	**29A SESSION KEYNOTE** A novel plant-microbiome co-culturing system reveals key associations of specific metabolites with plant growth and stress tolerance *Sanjay Swarup, National University of Singapore, Singapore*	Princess Alexia
11:15 a.m. – 11:40 a.m.	**29B** An untargeted LC-MS based work-flow for the structural characterization of biological polyesters *Rebecca Dauwe, Université de Picardie Jules Verne, France*	
11:40 a.m. – 11:55 a.m.	**29C** NMR-MS metabolomics reveals sulfonation in the Salicaceae *Clarice Noleto-Dias, Rothamsted Research, United Kingdom*	
10:45 a.m. – 12:00 p.m.	**Session 30:** Metabolite Identification 2 *(Session Chairs: Fidele Tugizimana & Christina Jones)*	
10:45 a.m. – 11:15 a.m.	**30A SESSION KEYNOTE** Correlation-based deconvolution (CorrDec) method for data-independent acquisition mass spectrometry *Ipputa Tada, Department of Genetics, SOKENDAI (Graduate University for Advanced Studies), Japan*	Princess Ariane
11:15 a.m. – 11:40 a.m.	**30B** Evaluation of molecular ionization propensities in different ionization modes: providing evidence for the presence of small molecules in synthetic blinded samples *Jamie Nunez, Pacific Northwest National Laboratory, United States*	
11:40 a.m. – 11:55 a.m.	**30C*** Improved oxylipins and fatty acids identification by using LC-DTIM-MS *Sonia Liggi, Department of Biochemistry and Cambridge Systems Biology Centre, University of Cambridge, United Kingdom*	
1:30 p.m. – 3:30 p.m.	**Plenary Session 4 and Closing Ceremony** *Jean-Charles Portais, University Toulouse, France*	