<table>
<thead>
<tr>
<th>Time</th>
<th>Day</th>
<th>Atlantic</th>
<th>Alexia</th>
<th>Ariane</th>
<th>Oceania Foyer</th>
</tr>
</thead>
<tbody>
<tr>
<td>11:00 a.m.</td>
<td>SUNDAY, JUNE 23</td>
<td>REGISTRATION OPEN</td>
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<tr>
<td>12:30 p.m. – 2:15 p.m.</td>
<td>W1: EMN – Data Fusion</td>
<td>W2: Mining the Metabolome</td>
<td>W3: Multi-Omics Integration &amp; Systems Metabolomics</td>
<td>W9: An Open-Source Pipeline for Appraisal of NMR Datasets</td>
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<tr>
<td>2:30 p.m. – 4:15 p.m.</td>
<td>W4: Application of Graphical Models to Metabolomics</td>
<td>W5: Plant Metabolomes: Natural &amp; Generated Variability</td>
<td>W6: How to Link Metabolome &amp; Genome Mining</td>
<td>W10: The Importance of Quality Assurance &amp; Quality Control</td>
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</tr>
<tr>
<td>4:30 p.m. – 6:15 p.m.</td>
<td>W7: EMN – Professional Career Development</td>
<td>W8: Putting Metabolomic Data into Context</td>
<td>W11: Towards FAIR Spectral Libraries</td>
<td>W16: Application Metabolomics in Industry</td>
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<tr>
<td>6:30 p.m. – 8:30 p.m.</td>
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<tr>
<td>7:30 a.m. – 10:15 a.m.</td>
<td>MONDAY, JUNE 24</td>
<td>REGISTRATION / INFO DESK OPEN</td>
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<tr>
<td>8:00 a.m. – 9:30 a.m.</td>
<td>Plenary Session 2</td>
<td>– Dorret Boomsma – King Willem-Alexander Hall</td>
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<tr>
<td>10:15 a.m. – 12:00 p.m.</td>
<td>LUNCH IN FOYER WITH EXHIBITS – PLATINUM SPONSOR PRESENTATIONS</td>
<td>Sponsor Pres: SCIEX</td>
<td>Sponsor Pres: Waters Corporation</td>
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<tr>
<td>12:20 p.m. – 1:20 p.m.</td>
<td></td>
<td>5. Metabolic Disease</td>
<td>6. Food Applications 1</td>
<td>7. Flux Studies</td>
<td>8. Novel Instruments, Tools and Services</td>
</tr>
<tr>
<td>5:30 p.m. – 7:00 p.m.</td>
<td>Poster Session 2 – Odd Numbers – Exhibit Foyer</td>
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<tr>
<td>7:00 p.m. – 8:00 p.m.</td>
<td>Metabolomics Society Town Hall Meeting</td>
<td>– Atlantic</td>
<td>– Odd Numbers – Exhibit Foyer</td>
<td>– Pacific</td>
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<tr>
<td>7:45 a.m.</td>
<td>TUESDAY, JUNE 25</td>
<td>REGISTRATION / INFO DESK OPEN</td>
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<tr>
<td>8:00 a.m.</td>
<td>Plenary Session 3</td>
<td>– Cathie Martin – King Willem-Alexander Hall</td>
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<tr>
<td>10:15 a.m. – 12:00 p.m.</td>
<td>LUNCH IN FOYER WITH EXHIBITS – PLATINUM SPONSOR PRESENTATIONS</td>
<td>Sponsor Pres: Thermo Fisher Scientific</td>
<td>Sponsor Pres: Shimadzu Europa GmbH</td>
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<tr>
<td>12:20 p.m. – 1:20 p.m.</td>
<td></td>
<td>17. Ageing and Disease</td>
<td>18. Food Applications 2</td>
<td>19. Data Integration &amp; Data Basing 2</td>
<td>20. Regulatory Session</td>
</tr>
<tr>
<td>5:30 p.m. – 7:00 p.m.</td>
<td>Poster Session 3 – Even Numbers – Exhibit Foyer</td>
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<tr>
<td>7:30 p.m. – 10:30 p.m.</td>
<td>Conference Dinner – Xiringuito</td>
<td>– Pacific</td>
<td>– Even Numbers – Exhibit Foyer</td>
<td>– Pacific</td>
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<tr>
<td>8:30 a.m.</td>
<td>WEDNESDAY, JUNE 26</td>
<td>REGISTRATION / INFO DESK OPEN</td>
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<tr>
<td>8:30 a.m. – 9:30 a.m.</td>
<td>Plenary Session 4</td>
<td>– Even Numbers – Exhibit Foyer</td>
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<tr>
<td>10:15 a.m. – 12:00 p.m.</td>
<td>LUNCH IN FOYER WITH EXHIBITS – PLATINUM SPONSOR PRESENTATIONS</td>
<td>Sponsor Pres: Bruker Daltonics/Bruker Biospin</td>
<td>Sponsor Pres: Agilent Technologies</td>
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<tr>
<td>12:20 p.m. – 1:20 p.m.</td>
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<td>29. Plant Applications 2</td>
<td>30. Metabolite Identification 2</td>
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<tr>
<td>1:30 p.m. – 3:30 p.m.</td>
<td>Plenary Session 4</td>
<td>– Jean-Charles Portais – Closing Ceremony</td>
<td>– King Willem-Alexander Hall</td>
<td>– Pacific</td>
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</tr>
<tr>
<td>4:30 p.m. – 6:15 p.m.</td>
<td>W12: Dynamic Modeling of Human Metabolism</td>
<td>W13: Beyond pathway mapping</td>
<td>W14: Standardizing the Fluxomics Workflows</td>
<td>W15: Tools to Study the Microbiome-Metabolome Interplay</td>
<td>W17: Data Integration &amp; Data Basing 2</td>
</tr>
<tr>
<td>6:30 p.m. – 8:30 p.m.</td>
<td>W18: EMN – Volatomics in Human Health</td>
<td>W19: Metabolic Disease</td>
<td>W20: Microbial Applications</td>
<td>W21: Metabolite Identification 2</td>
<td>W22: Plant Metabolomes: Natural &amp; Generated Variability</td>
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### Monday, June 24

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Location</th>
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<tbody>
<tr>
<td>3:30 p.m.–5:00 p.m.</td>
<td>Opening Ceremony and Plenary Session 1</td>
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<td></td>
<td><em>Joshua Rabinowitz, Lewis-Sigler Institute, United States</em></td>
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### Tuesday, June 25

<table>
<thead>
<tr>
<th>Time</th>
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<tbody>
<tr>
<td>8:30 a.m.–9:30 a.m.</td>
<td>Plenary Session 2</td>
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<td><em>Dorret I. Boomsma, Netherlands Twin Register, Vrije Universiteit, Netherlands</em></td>
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#### Session 1: Cancer
*(Session Chairs: Hunter Moseley & Maria Eugenia Monge)*

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<tr>
<th>Time</th>
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</table>
| 10:15 a.m.–12:00 p.m. | *1A SESSION KEYNOTE* Metabolomics Applications for Oncology and Immunology in Drug Discovery  
*Thomas Roddy, Agios Pharmaceuticals, United States* |                                               |
| 10:15 a.m.–10:45 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* |                                               |
| 10:45 a.m.–11:20 a.m. | *1C Investigating the metabolic response of cancer cells to indisulam  
*Lili Herendi, PhD student, United Kingdom* | Atlantic                                       |
| 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* |                                               |

#### Session 2: Plant Applications 1
*(Session Chairs: Sanjay Swarup & Jasen Finch)*

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<th>Time</th>
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| 10:15 a.m.–12:00 p.m. | *2A SESSION KEYNOTE* The volatile flavor composition network in tomato and its modification  
*Antonio Granell, CSIC, Spain* |                                               |
| 10:15 a.m.–10:45 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* | King Willem Alexander                           |
| 10:45 a.m.–11:05 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* |                                               |
| 11:05 a.m.–11:20 a.m. | *2D Chocolate metabolomics  
*Robert Hall, Wageningen UR, Netherlands* |                                               |
| 11:20 a.m.–11:40 a.m. | *2E A tissue specific metabolomic study in hybrid aspen  
*Iłara Budzinski, Swedish University of Agricultural Sciences (SLU), Sweden* |                                               |
**NEW FRONTIERS**

**AWARD WINNERS**

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<tr>
<th>Time</th>
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</table>
| **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 |                     |
| 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 | Princess Alexia      |
| 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 |                     |
| 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 | Princess Ariane     |
| 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 |                     |
<table>
<thead>
<tr>
<th>Time</th>
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<tbody>
<tr>
<td>1:30 p.m. – 3:15 p.m.</td>
<td><strong>Session 5: Metabolic Disease</strong> <em>(Session Chairs: Christophe Junot &amp; Katharina Herzog)</em></td>
</tr>
</tbody>
</table>
| 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 |
| 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 |

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<tr>
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<tr>
<td>1:30 p.m. – 3:15 p.m.</td>
<td><strong>Session 6: Food Applications 1</strong> <em>(Session Chairs: Cristina Andres Lacueva &amp; Jessica Cooperstone)</em></td>
</tr>
</tbody>
</table>
| 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 |
| 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 |
## Tuesday, June 25

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
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<tbody>
<tr>
<td>1:30 p.m. – 3:15 p.m.</td>
<td><strong>Session 7:</strong> Flux Studies (Session Chairs: Barbara Bakker &amp; Bekzod Khakimov)</td>
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</tbody>
</table>
| 1:30 p.m. – 2:30 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 Cascente, University of Barcelona, Spain* |                |
| 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* | Princess Alexia |
| 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, IISP, Spain* |                |
| 1:30 p.m. – 3:15 p.m. | **Session 8:** Novel Instrumentations, Tools and Services (Presented by Platinum and Gold Sponsors)        |                |
| 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**  
*Bioclades 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 |                |
**Session 9: Epidemiology**  
*(Session Chairs: Krista Zanetti & Julie Schmidt)*

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| 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* | |

**Session 10: Microbial Applications**  
*(Session Chairs: Adriana Carvalho de Souza & Douglas McCloskey)*

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| 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* | **AWARD WINNERS**
## Tuesday, June 25

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| **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 |                  |
| 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 | Princess Alexia |
| 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 |                  |
| 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 | Princess Ariane |
| 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 |                  |
## Wednesday, June 26

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<tr>
<td>8:30 a.m. – 9:30 a.m.</td>
<td>Plenary Session 2</td>
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<td>Cathie Martin, John Innes Centre, Colney Research Park, UK</td>
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<tr>
<td>10:15 a.m. – 12:00 p.m</td>
<td><strong>Session 13: Lipidomics and Cardiovascular Disease</strong> (Session Chairs: Jules Griffin &amp; Aline Martins)</td>
<td>Atlantic</td>
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<tr>
<td>10:15 a.m. – 10:45 a.m.</td>
<td><strong>13A SESSION KEYNOTE</strong></td>
<td>Atlantic</td>
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<td>High-throughput lipidomic quantitation of human blood in cancer screening</td>
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<td>Michal Holcapek, University of Pardubice, Czech Republic</td>
<td>Atlantic</td>
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<td>10:45 a.m. – 11:05 a.m.</td>
<td><strong>13B</strong></td>
<td>Atlantic</td>
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<td>Changes in plasma lipids predict pravastatin efficacy in secondary prevention</td>
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<td>Peter Meikle, Baker Heart and Diabetes Institute, Australia</td>
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<td>11:05 a.m. – 11:20 a.m.</td>
<td><strong>13C</strong></td>
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<td>Metabolomics analysis of human atherosclerotic plaques reveals a potential novel pathway of macrophage foam cell apoptosis in advanced atherosclerosis</td>
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<td>Panagiotis Vorkas, Imperial College London, United Kingdom</td>
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<td>11:20 a.m. – 11:40 a.m.</td>
<td><strong>13D</strong></td>
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<td>Plasma metabolomics profiles associated with endothelial health and dysfunction impose changes to endothelial glycan biosynthesis and reflect endothelial catecholamine response</td>
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<td>Óttar Rolfsson, University of Iceland, Iceland</td>
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<td>11:40 a.m. – 11:55 a.m.</td>
<td><strong>13E</strong></td>
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<td>Sphingolipidomics investigation of the ischemic brain injury</td>
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<td>Ching-Hua Kuo, National Taiwan University, Taiwan</td>
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<td>10:15 a.m. – 12:00 p.m.</td>
<td><strong>Session 14: Plant Defense</strong></td>
<td>King Willem Alexander</td>
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<td><em>(Session Chairs: Annick Moing &amp; Halford Dace)</em></td>
<td>King Willem Alexander</td>
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<td>10:15 a.m. – 10:45 a.m.</td>
<td><strong>14A SESSION KEYNOTE</strong></td>
<td>King Willem Alexander</td>
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<td>Elucidating insect resistance in tomato through genetical metabolomics</td>
<td>King Willem Alexander</td>
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<td>Ric de Vos, Bioscience, Wageningen Plant Research, Wageningen University and Research, Netherlands</td>
<td>King Willem Alexander</td>
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<td>10:45 a.m. – 11:05 a.m.</td>
<td><strong>14B</strong></td>
<td>King Willem Alexander</td>
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<td>Dissecting the Genetic Basis of Variation in Tomato Fruit Metabolism and Pathogen Resistance through Multimodal Investigation of Wild SpeciesIntrogressions</td>
<td>King Willem Alexander</td>
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<td>Jedrzej Szymanski, Leibniz Institute of Plant Genetics and Crop Plant Research, Germany</td>
<td>King Willem Alexander</td>
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<td>11:05 a.m. – 11:20 a.m.</td>
<td><strong>14C</strong></td>
<td>King Willem Alexander</td>
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<td>Metabolomics application to unravel the biochemistry underlying enhancement of drought stress tolerance in crops by plant growth promoting rhizobacteria</td>
<td>King Willem Alexander</td>
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<td>Fidele Tugizimana, University of Johannesburg, South Africa</td>
<td>King Willem Alexander</td>
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<td>11:20 a.m. – 11:40 a.m.</td>
<td><strong>14D</strong></td>
<td>King Willem Alexander</td>
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<td>A strategy for the discovery and characterisation of health and decline biomarkers in British Oak trees using non-targeted metabolomics</td>
<td>King Willem Alexander</td>
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<td>Jasen Finch, Aberystwyth University, United Kingdom</td>
<td>King Willem Alexander</td>
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<td>11:40 a.m. – 11:55 a.m.</td>
<td><strong>14E</strong></td>
<td>King Willem Alexander</td>
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<td>Linking the volatilome and metabolome via plant defenses: stimulation of the salicylic acid pathway recruits natural enemies below ground</td>
<td>King Willem Alexander</td>
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<td>Camila Filgueiras, Cornell University, United States</td>
<td>King Willem Alexander</td>
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<td><strong>10:15 a.m. – 12:00 p.m.</strong></td>
<td><strong>Session 15: Data Analysis &amp; Statistics</strong> <em>(Session Chairs: Age Smilde &amp; Isabel Orf)</em></td>
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| 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* |          |
| 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* | Princess Alexia |
| 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* |          |
| 10:45 a.m. – 11:05 a.m. | **16B**  
Comprehensive Single Cell Multi Omics  
*Christian Berchtold, Institute for Chemistry and Bioanalytics, Switzerland* | Princess Ariane |
| 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* |          |
### Session 17: Ageing and Disease

*Session Chairs: Matej Oresic & Candice Ulmer*

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| 1:30 p.m. – 2:00 p.m. | **17A SESSION KEYNOTE**
Multimomic 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* |              |

### Session 18: Food Applications 2

*Session Chairs: Sastia Putri & Johanna Jokioja*

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| 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

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<th>Time</th>
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<tr>
<td><strong>1:30 p.m. – 3:15 p.m.</strong></td>
<td><strong>Session 19: Data Integration &amp; Data Basing 2</strong> <em>(Session Chairs: Dan Raftery &amp; Dara Daygon)</em></td>
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| 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* |                        |
| 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* | Princess Alexa          |
| 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* |                        |

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| **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* |                        |
| 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* | Princess Ariane         |
| 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* |                        |
<p>| 2:50 p.m. – 3:15 p.m. | *<em>Panel Discussion with all presenters, moderated by Pim Leonards</em> |                        |</p>
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<tr>
<td>3:45 p.m. – 5:30 p.m.</td>
<td><strong>Session 21: Infection and Immunity</strong> <em>(Session Chairs: Darren Creek &amp; Xinzhu Wang)</em></td>
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| 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 |                  |
| 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 | Atlantic         |
| 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 |                  |
| 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 | King Willem Alexander |
| 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 |                  |
### Wednesday, June 26

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| 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* |                  |
| 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* | Princess Alexia |
| 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* |                  |
| 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* | Princess Ariane |
| 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* |                  |
### Thursday, June 27

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| 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 |                   |
| 9:15 a.m. – 9:40 a.m. | **25B**  
Comprehensive metabolomic and immunological profiling of Asthma COPD Overlap (ACO)  
Nilanjana Ghosh, School of Medical Science and Technology, India | Atlantic          |
| 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 |                   |
| 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 | Princess Alexia |
| 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 |                   |
| 9:15 a.m. – 9:40 a.m. | **27B**  
Metabolic footprint of Parkinson’s Disease: integration of patient-derived X-omics data with a human genome-scale model.  
Agnieszka Wegrzyn, LACDR, Leiden University, Netherlands | Princess Ariane  |
| 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 |                   |
## Thursday, June 27

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