18th Annual Conference of the Metabolomics Society

METABOLOMICS 2022

Valencia, Spain  |  JUNE 19-23

SCHEDULE OF ORAL PRESENTATIONS
## SUNDAY, JUNE 19

<table>
<thead>
<tr>
<th>Time</th>
<th>Auditorium 2</th>
<th>MP 1 – AB</th>
<th>MP 1 – CD</th>
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<tbody>
<tr>
<td>11:00 a.m.</td>
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<tr>
<td>12:00 p.m. – 2 p.m.</td>
<td>W1: Ion Mobility in Metabolomics: New Tech and Workflows</td>
<td>W2: Spectra Processing Using MetaboAnalyst 5.0 Part I</td>
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<tr>
<td>2:15 p.m. – 4:15 p.m.</td>
<td>W3: Mass Spectrometry Data Processing with MZmine 3</td>
<td>W2 Cont: Spectra Processing Using MetaboAnalyst 5.0 Part 2</td>
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<tr>
<td>4:30 p.m. – 6:30 p.m.</td>
<td>W5: State of QA/QC Best Practices in LC-MS-Based Untargeted Metabolomics</td>
<td>W6: EMN Professional Career Development</td>
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<td>6:30 p.m. – 8:30 p.m.</td>
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<td>Career Night</td>
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## MONDAY, JUNE 20

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<tr>
<th>Time</th>
<th>Auditorium 2</th>
<th>MP 1 – AB</th>
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<tr>
<td>7:45 a.m.</td>
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<tr>
<td>8:30 a.m. – 10:15 a.m.</td>
<td>W8: Clinical Lipidomics</td>
<td>W9: Mining the Metabolome using the Mass Spec Query</td>
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<tr>
<td>10:30 a.m. – 12:30 p.m.</td>
<td>W11: The 3 R’s of Effective Data Sharing in Metabolomic Epidemiology</td>
<td>W12: Revisiting CASMI: compound ID for 500 new unknowns, using LC-MS/MS data</td>
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<tr>
<td>1:30 p.m. – 3 p.m.</td>
<td>Auditorium 2</td>
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<tr>
<td>3 p.m. – 3:30 p.m.</td>
<td>Auditorium 1</td>
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<tr>
<td>3:30 p.m. – 5:30 p.m.</td>
<td>W1: Epidemiology</td>
<td>1 Epidemiology</td>
<td>2 Computational Metabolomics Workflows</td>
</tr>
<tr>
<td>5:15 p.m. – 6:45 p.m.</td>
<td>W2: Metabolomics Society Town Hall Meeting</td>
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<td>6:30 p.m. – 8:30 p.m.</td>
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</table>

## TUESDAY, JUNE 21

<table>
<thead>
<tr>
<th>Time</th>
<th>Auditorium 1</th>
<th>Auditorium 2</th>
<th>MP 1</th>
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<tbody>
<tr>
<td>7:45 a.m.</td>
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<tr>
<td>8:30 a.m. – 9:30 a.m.</td>
<td>W6: Neurological Disorders</td>
<td>4 Neurological Disorders</td>
<td>5 Data Analysis and Modeling</td>
</tr>
<tr>
<td>9:30 a.m. – 10:15 a.m.</td>
<td>W13: Data Analysis and Modeling</td>
<td>5 Data Analysis and Modeling</td>
<td>6 Plant Metabolomics</td>
</tr>
<tr>
<td>10:15 a.m. – 12 p.m.</td>
<td>W14: Cancer</td>
<td>13 Cancer</td>
<td>14 Collaborative Data Science &amp; Cloud Computing</td>
</tr>
<tr>
<td>12 p.m. – 1:30 p.m.</td>
<td>W15: Poster Session 2</td>
<td>15 Technology Advancements II</td>
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<tr>
<td>12:30 p.m. – 12:50 p.m.</td>
<td>Sponsor Pres: Bruker</td>
<td>Sponsor Pres: SCIEX</td>
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<tr>
<td>1:30 p.m. – 3 p.m.</td>
<td>7 Infectious Diseases</td>
<td>8 MetID I</td>
<td>9 Technology Advancements I</td>
</tr>
<tr>
<td>3 p.m. – 3:30 p.m.</td>
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<tr>
<td>3:30 p.m. – 5 p.m.</td>
<td>W16: Lipidomics and Cardiovascular Diseases</td>
<td>10 Lipidomics and Cardiovascular Diseases</td>
<td>11 Vendor Session</td>
</tr>
<tr>
<td>5 p.m. – 6:30 p.m.</td>
<td>W17: Poster Session 3</td>
<td>12 Plant and Environmental Applications I</td>
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<tr>
<td>6:45 p.m. – 8:15 p.m.</td>
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## WEDNESDAY, JUNE 22

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<th>Time</th>
<th>Auditorium 1</th>
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<td>8:00 a.m.</td>
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<tr>
<td>8:30 a.m. – 9:30 a.m.</td>
<td>W18: Plenary Session 3 – Asaph Aharoni</td>
<td>13 Cancer</td>
<td>14 Collaborative Data Science &amp; Cloud Computing</td>
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<tr>
<td>9:30 a.m. – 10:15 a.m.</td>
<td>W19: Poster Session 4</td>
<td>15 Technology Advancements II</td>
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<tr>
<td>10:15 a.m. – 12 p.m.</td>
<td>W20: Cancer</td>
<td>16 Cancer</td>
<td>17 Plant and Environmental Applications II</td>
</tr>
<tr>
<td>12 p.m. – 1:30 p.m.</td>
<td>W21: Poster Session 5</td>
<td>18 QA/QC and Reproducibility</td>
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<tr>
<td>12:30 p.m. – 1:20 p.m.</td>
<td>Sponsor Pres: Agilent</td>
<td>Sponsor Pres: Thermo Fisher Scientific</td>
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<tr>
<td>1:30 p.m. – 3 p.m.</td>
<td>19 Metabolomics Throughout the Lifecourse</td>
<td>19 Metabolomics Throughout the Lifecourse</td>
<td>20 MetID II</td>
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<tr>
<td>3 p.m. – 3:30 p.m.</td>
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<tr>
<td>3:30 p.m. – 5:15 p.m.</td>
<td>W22: Poster Session 6</td>
<td>21 Metabolic Diseases</td>
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<td>5:15 p.m. – 6:45 p.m.</td>
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<td>7:30 p.m. – 10:30 p.m.</td>
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## THURSDAY, JUNE 23

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<th>Time</th>
<th>Auditorium 1</th>
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<tbody>
<tr>
<td>8:15 a.m.</td>
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<tr>
<td>8:30 a.m. – 10:15 a.m.</td>
<td>W23: Microbiome and Gastrointestinal Function</td>
<td>22 Microbiome and Gastrointestinal Function</td>
<td>23 Natural Products</td>
</tr>
<tr>
<td>10:15 a.m. – 11:30 a.m.</td>
<td>W24: Analytical Methods in Lipidomics</td>
<td>24 Analytical Methods in Lipidomics</td>
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</tr>
<tr>
<td>11:30 a.m. – 1 p.m.</td>
<td>W25: Poster Session 4</td>
<td>25 Poster Session 4</td>
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<td>1 p.m.</td>
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</tbody>
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**AGENDA AT A GLANCE**

- Metabolomics in Health and Disease
- Computational Metabolomics, Statistics & Bioinformatics
- Plants, Food, Environment and Microbes
- Technology Advancements

**REGISTRATION**

- SUNDAY, JUNE 19:
  - 11:00 a.m.
  - 12:00 p.m. – 2 p.m.
  - 2:15 p.m. – 4:15 p.m.
  - 4:30 p.m. – 6:30 p.m.
  - 6:30 p.m. – 8:30 p.m.

- MONDAY, JUNE 20:
  - 7:45 a.m.
  - 8:15 a.m. – 10:15 a.m.
  - 10:30 a.m. – 12:30 p.m.
  - 1:30 p.m. – 3 p.m.
  - 3:30 p.m. – 5:30 p.m.
  - 5:15 p.m. – 6:45 p.m.
  - 6:30 p.m. – 8:30 p.m.

- TUESDAY, JUNE 21:
  - 7:45 a.m.
  - 8:30 a.m. – 9:30 a.m.
  - 9:30 a.m. – 10:15 a.m.
  - 10:15 a.m. – 12 p.m.
  - 12 p.m. – 1:30 p.m.
  - 12:30 p.m. – 12:50 p.m.
  - 1:30 p.m. – 3 p.m.
  - 3 p.m. – 3:30 p.m.
  - 3:30 p.m. – 5 p.m.
  - 5 p.m. – 6:30 p.m.
  - 6:45 p.m. – 8:15 p.m.

- WEDNESDAY, JUNE 22:
  - 8:00 a.m.
  - 8:30 a.m. – 9:30 a.m.
  - 9:30 a.m. – 10:15 a.m.
  - 10:15 a.m. – 12 p.m.
  - 12 p.m. – 1:30 p.m.
  - 12:30 p.m. – 1:20 p.m.
  - 1:30 p.m. – 3 p.m.
  - 3 p.m. – 3:30 p.m.
  - 3:30 p.m. – 5:15 p.m.
  - 5:15 p.m. – 6:45 p.m.
  - 7:30 p.m. – 10:30 p.m.

- THURSDAY, JUNE 23:
  - 8:15 a.m.
  - 8:30 a.m. – 10:15 a.m.
  - 10:15 a.m. – 11:30 a.m.
  - 11:30 a.m. – 1 p.m.
  - 1 p.m.
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Abstract #</th>
</tr>
</thead>
</table>
| 1:30 p.m. – 3 p.m. | **Welcome and Opening Plenary Session 1** Molecular imaging in metabolomics: single cells and beyond  
*Ron Heeren, Maastricht University, Netherlands* | Auditorium 1 |
| 3:30 p.m. – 5:15 p.m. | **Session 1. Epidemiology**  
*Session Chairs: Krista Zanetti and Nicholas Rattray* | Auditorium 2 |
| 3:30 p.m. – 4 p.m. | **1.1 KEYNOTE** Metabolic view on sex differences and health risk: Metabolome-wide association studies  
*Julijana Ivanisevic, University of Lausanne, Switzerland* | 421 |
| 4 p.m. – 4:20 p.m. | **1.2** Integrated plasma and cerebrospinal fluid multi-omics relate to the AT(N) framework and genetic risk for Alzheimer’s disease  
*Jin Xu, King’s College London, United Kingdom* | 94 |
| 4:20 p.m. – 4:35 p.m. | **1.3** Novel plasma metabolomic markers associated with diabetes progression in older Puerto Ricans  
*Shilpa Bhupathiraju, Harvard Medical School, United States* | 246 |
| 4:35 p.m. – 4:55 p.m. | **1.4** Lipoprotein and metabolite associations to breast cancer risk in the HUNT2 study  
*Julia Debi, Norwegian University of Science and Technology, Norway* | 159 |
| 4:55 p.m. – 5:10 p.m. | **1.5** COMETS Analytics v2.0 implements generalized linear models: Findings from the COnsortium of METabolomics Studies (COMETS) Lung Disease Interest Group  
*Rachel Kelly, Harvard Medical School, United States* | 238 |
| 3:30 p.m. – 5:15 p.m. | **Session 2. Computational Metabolomics Workflows**  
*Session Chairs: Ewy Mathe and Steffen Neumann* | Auditorium 1 |
| 3:30 p.m. – 4 p.m. | **2.1 KEYNOTE** MS-DIAL 5 for EAD-based untargeted metabolomics and lipidomics  
*Hiroshi Tsugawa, Tokyo University of Agriculture and Technology, Japan* | 431 |
| 4 p.m. – 4:20 p.m. | **2.2** Amanida meta-analysis approach: metabolomics results combination for clinical applications  
*Maria Llambrich, Universitat Rovira I Virgili, Spain* | 78 |
| 4:20 p.m. – 4:35 p.m. | **2.3** QualiMon LaMa – Live quality monitoring in non-targeted analysis using LandMark features  
*Carl Brunius, Chalmers University Of Technology, Sweden* | 80 |
| 4:35 p.m. – 4:55 p.m. | **2.4** Adding clinical value to the 1H NMR metabolomics data by new spectral processing algorithms/software  
*Panteleimon Takis, Imperial College London, United Kingdom* | 286 |
| 4:55 p.m. – 5:10 p.m. | **2.5** Processing of small molecule gas chromatography–mass spectrometry data in Galaxy  
*Helge Hecht, RECETOX, Czech Republic* | 277 |
### Monday, June 20

<table>
<thead>
<tr>
<th>Time</th>
<th>Session 3. Foodomics</th>
<th>Session Chairs: Kati Hanhineva and Kang Chen</th>
<th>Abstract #</th>
</tr>
</thead>
<tbody>
<tr>
<td>3:30 p.m. – 5:15 p.m.</td>
<td>3.1 KEYNOTE</td>
<td>Untargeted Metabolomics as a valuable Tool for quality Improvement of Fine-flavor cocoa and Coffee beverages during food processing</td>
<td>471</td>
</tr>
<tr>
<td></td>
<td>Monica Cala, Universidad de Los Andes, Colombia</td>
<td>Multi Purpose 1</td>
<td></td>
</tr>
<tr>
<td>3:30 p.m. – 4 p.m.</td>
<td>3.2</td>
<td>Metabolomics reveals the chemical dynamics in green and white asparagus</td>
<td>282</td>
</tr>
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<td></td>
<td>Robert Hall, Wageningen University &amp; Research, Netherlands</td>
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</tr>
<tr>
<td>4 p.m. – 4:20 p.m.</td>
<td>3.3</td>
<td>Application of FTIR spectroscopy in tandem with machine learning for the microbiological quality assessment and discrimination of various types of mussels</td>
<td>335</td>
</tr>
<tr>
<td></td>
<td>Anastasia Lytou, Agricultural University Of Athens, Greece</td>
<td></td>
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<tr>
<td>4:20 p.m. – 4:35 p.m.</td>
<td>3.4</td>
<td>Lipidomic profiling of bioactive lipids during spontaneous fermentation of fine-flavour cocoa</td>
<td>215</td>
</tr>
<tr>
<td></td>
<td>Miguel Fernández-Niño, Leibniz Institute of Plant Biochemistry: Halle Neustadt, DE, Colombia</td>
<td></td>
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<tr>
<td>4:35 p.m. – 4:55 p.m.</td>
<td>3.5</td>
<td>A foodomics study on the molecular composition of cooking vapor from the processing of foodstuff</td>
<td>64</td>
</tr>
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<td></td>
<td>Leopold Weidner, Technical University Of Munich, Germany</td>
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<tr>
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| **8:30 a.m. – 9:30 a.m.** | Plenary Session 2  
Metabolomics and women’s reproductive, pregnancy and perinatal health  
*Deborah Lawlor, University Of Bristol, United Kingdom* | Auditorium 1 |
| **10:15 a.m. – 12 noon** | **Session 4. Neurological Disorders**  
Session Chairs: Tuulia Hyötyläinen and Sofina Begum | Auditorium 1 |
| 10:15 a.m. – 10:45 a.m. | **4.1 SESSION KEYNOTE**  
Immune activation, neurodevelopment, and risk of offspring ADHD: a survey of the circulating maternal metabolome during pregnancy  
*Su Chu, Brigham and Women’s Hospital and Harvard Medical School, United States* | 340 |
| 10:45 a.m. – 11:05 a.m. | **4.2**  
The circulating metabolome associates with severity of acute traumatic brain injury, computed tomography findings, and patient outcomes  
*Matej Oresic, Örebro University, Sweden* | 267 |
| 11:05 a.m. – 11:20 a.m. | **4.3**  
Novel CSF biomarkers of GLUT1 deficiency syndrome: implications beyond the brain’s energy deficit  
*Tessa Peters, Radboudumc, Netherlands* | 87 |
| 11:20 a.m. – 11:40 a.m. | **4.4**  
Identification of neurodegeneration indicators and disease progression in metachromatic leukodystrophy using quantitative NMR-based urinary metabolomics  
*Christoph Trautwein, University Of Tuebingen, Germany* | 330 |
| 11:40 a.m. – 11:55 a.m. | **4.5**  
Targeted Metabolomic and Lipidomic Analysis in Parkinson’s Disease Brain Tissue Across Spectrum of Cognitive Impairment  
*Karel Kalecký, Baylor University, United States* | 360 |
| **10:15 a.m. – 12 noon** | **Session 5. Data Analysis and Modeling**  
Session Chairs: Serge Rudaz and Yann Guitton | Auditorium 2 |
| 10:15 a.m. – 10:45 a.m. | **5.1 KEYNOTE**  
Democratizing metabolomics through new-generation computing framework  
*Jianguo (Jeff) Xia, McGill University, Canada* | 422 |
| 10:45 a.m. – 11:05 a.m. | **5.2**  
FAMetA: a mass-isototopogue-based tool for the comprehensive analysis of fatty acid metabolism  
*Juan Carlos García Cañaveras, IIS-La Fe, Spain* | 265 |
| 11:05 a.m. – 11:20 a.m. | **5.3**  
Performance evaluation and applicability of single-sample pathway analysis methods to metabolomics data  
*Cecilia Wieder, Imperial College London, United Kingdom* | 102 |
| 11:20 a.m. – 11:40 a.m. | **5.4**  
XomicsToModel: Multiomic data integration and generation of thermodynamically consistent metabolic models  
*Ronan Fleming, Leiden University, Netherlands* | 42 |
| 11:40 a.m. – 11:55 a.m. | **5.5**  
Inferring causal linkages in longitudinal omics studies using econometric tools  
*Gerard Bryan Gonzales, Wageningen University, Netherlands* | 57 |
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
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</tr>
</thead>
<tbody>
<tr>
<td>10:15 a.m. – 12 noon</td>
<td><strong>Session 6. Plant Metabolomics</strong>&lt;br&gt;<em>Session Chairs: Robert Hall and Carla Antonio</em></td>
<td>Multi Purpose 1</td>
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<tr>
<td>10:15 a.m. – 10:45 a.m.</td>
<td>6.1 KEYNOTE &lt;br&gt;HPTLC application to metabolomics as a supplementary tool for in-silica identification&lt;br&gt;<em>Young Hae Choi, Institute of Biology, Leiden University, Netherlands</em></td>
<td>418</td>
</tr>
<tr>
<td>10:45 a.m. – 11:05 a.m.</td>
<td>6.2 Combining Metabolomics and Phenomics approach to determinate horticultural plant stress response under different conditions&lt;br&gt;<em>Paolo Bonini, oloBion, Spain</em></td>
<td>235</td>
</tr>
<tr>
<td>11:05 a.m. – 11:20 a.m.</td>
<td>6.3 SISSSH silencing reveals specific pathogen-triggered salicylic acid metabolism in tomato&lt;br&gt;<em>Celia Payá, IBMCP, Spain</em></td>
<td>97</td>
</tr>
<tr>
<td>11:20 a.m. – 11:40 a.m.</td>
<td>6.4 Multi-Omics Analysis Provides Insights into the Acclimation of Plants to High-light Stress&lt;br&gt;<em>Gerd U. Balcke, Leibniz-Institute of Plant Biochemistry, Deutschland</em></td>
<td>284</td>
</tr>
<tr>
<td>11:40 a.m. – 11:55 a.m.</td>
<td>6.5 Mass spectrometry imaging allows plant metabolome changes in response to mycotoxin accumulation to be spatially resolved&lt;br&gt;<em>Laura Righetti, Food and Drug Department, University of Parma, Italy</em></td>
<td>135</td>
</tr>
<tr>
<td>12:20 p.m. – 1:20 p.m.</td>
<td><strong>Sponsor Lunch Presentations</strong></td>
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<td><strong>Bruker</strong>&lt;br&gt;Title TBD&lt;br&gt;Presenter TBD</td>
<td>Auditorium 1</td>
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<td><strong>SCIEX</strong>&lt;br&gt;Qualitative flexibility combined with quantitative power using the ZenoTOF 7600 system&lt;br&gt;<em>Jean-Baptiste Vincendet, Sr Market Development Manager, SCIEX</em></td>
<td>Auditorium 2</td>
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## Tuesday, June 21

<table>
<thead>
<tr>
<th>Time</th>
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</thead>
</table>
| 1:30 p.m. – 3 p.m. | Session 7. Infectious Diseases  
*Session Chairs: Jessica Lasky-Su and Karl Burgess* | Auditorium 1 |
| 1:30 p.m. – 1:50 p.m. | 7.1 Genome-scale metabolic model reveals long-term antiretroviral treatment-induced system-level metabolic shift towards oxidative phosphorylation in HIV-infection  
Ujjwal Neogi, Karolinska Institutet, Sweden | 162 |
| 1:50 p.m. – 2:05 p.m. | 7.2 Untargeted metabolomics by capillary electrophoresis-mass spectrometry of human pulmonary TB tissue identified polyamine biosynthesis as a potential host-directed therapeutic target  
Carolina Gonzalez-Riano, Centro de Metabolómica y Bioanálisis (CEMBIO) Facultad de Farmacia, Universidad San Pablo-CEU, CEU Universities, Spain | 119 |
| 2:05 p.m. – 2:25 p.m. | 7.3 Metabolic clustering of individuals prior to COVID-19 infection identifies a severe COVID-19 cluster that is recapitulated with samples during and after infection  
Kevin Mendez, Harvard Medical School, United States | 149 |
| 2:25 p.m. – 2:40 p.m. | 7.4 Profiling metabolites and lipoproteins in COMETA, an Italian cohort of COVID-19 patients  
Gaia Meoni, University of Florence, Italy | 274 |
| 2:40 p.m. – 3 p.m. | 7.5 Metabolic adaptation of Staphylococcus epidermidis biofilms to nitric oxide generated by the innate immune system  
Sandra Carvalho, Universidade Nova de Lisboa (ITQB NOVA), Portugal | 169 |
| 1:30 p.m. – 3 p.m. | Session 8. MetID I  
*Session Chairs: Oliver Fiehn and Maria Vinaixa* | Auditorium 2 |
| 1:30 p.m. – 1:50 p.m. | 8.1 An ensemble deep-learning spectral prediction model for metabolite annotation  
Soha Hassoun, Tufts University, United States | 365 |
| 1:50 p.m. – 2:05 p.m. | 8.2 TurboPutative: a web server for data handling and metabolite classification in untargeted metabolomics  
Rafael Barrero-Rodriguez, Spanish National Center for Cardiovascular Research (CNIC), Spain | 103 |
| 2:05 p.m. – 2:25 p.m. | 8.3 qHERMES: a molecular-formula-oriented method to target and quantify the metabolome  
Oscar Yanes, CIBERDEM & Universitat Rovira i Virgili & IISPV, Spain | 208 |
| 2:25 p.m. – 2:40 p.m. | 8.4 Reliable and fast MS/MS spectral-based analogue search with MS2Query  
Niek De Jonge, Wageningen University And Research (WUR), Netherlands | 334 |
| 2:40 p.m. – 3 p.m. | 8.5 MetFID: Convolutional Neural Network-Based Compound Fingerprint Prediction Tool for Metabolite Annotation  
Habtom Ressom, Georgetown University, United States | 279 |
## Tuesday, June 21

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Abstract #</th>
</tr>
</thead>
</table>
| 1:30 p.m. – 3 p.m. | **Session 9. Technology Advancements I**  
*Session Chairs: Leo Cheng and Guillermo Quintás* | Multi Purpose 1 |
| 1:30 p.m. – 1:50 p.m. | 9.1 Subcellular metabolomics – lessons learned from a compartment-specific metabolic investigation in a mouse model of Leigh syndrome  
*Roan Louw, North-West University, South Africa* | 420 |
| 1:50 p.m. – 2:05 p.m. | 9.2 A new method for the analysis of short-chain fatty acids (SCFA) and other polar metabolites in microbiome-related samples by ion-exchange chromatography-mass spectrometry (IC-MS)  
*Mariya Misheva, University Of Oxford, United Kingdom* | 203 |
| 2:05 p.m. – 2:25 p.m. | 9.3 Stool metabolome of four NIST stool reference material  
*Raquel Cumeras, Universitat Rovira i Virgili, Spain* | 115 |
| 2:25 p.m. – 2:40 p.m. | 9.4 Development of a High-Coverage and Quantitative Metabolomics Assay for Targeted Analysis of Multiple Pathways  
*Shuang Zhao, The Metabolomics Innovation Centre (TMIC), Canada* | 336 |
| 2:40 p.m. – 3 p.m. | 9.5 Extending the Scope of IH NMR Based Blood Metabolomics for the Analysis of Labile Antioxidants: Reduced and Oxidized Glutathione  
*G. A. Nagana Gowda, University Of Washington, United States* | 278 |
| 3:30 p.m. – 5 p.m. | **Session 10. Lipidomics and Cardiovascular Diseases**  
*Session Chairs: Jules Griffin and Stefania Noerman* | Auditorium 1 |
| 3:30 p.m. – 3:50 p.m. | 10.1 Lipidomic Latent Features Mediate Genetic Contributions to Coronary Heart Disease Risk: The Multi-Ethnic Study of Atherosclerosis (MESA)  
*David Herrington, Wake Forest University School Of Medicine, United States* | 304 |
| 3:50 p.m. – 4:05 p.m. | 10.2 Using OMICs to explore underlying pathways linking persistent organic pollutant exposures to cardiovascular disease in the Swedish Mammography Cohort  
*Yingxiao YAN, Chalmers University of Technology, Sweden* | 77 |
| 4:05 p.m. – 4:25 p.m. | 10.3 Lipidomics and flaxomics analysis reveals a novel role for fatty acid synthase in cholesterol and glycerolipid synthesis regulation in vivo.  
*Mikhail Golovko, UND, United States* | 288 |
| 4:25 p.m. – 4:40 p.m. | 10.4 Metabolomics and lipidomics at the top: Characterizing hypoxic responses of dwellers living permanently in La Rinconnada, the highest city of the world (5100m)  
*Jean-Charles Martin, INRAE, France* | 185 |
| 4:40 p.m. – 5 p.m. | 10.5 Targeted metabolomic profiles among genetically confirmed familial hypercholesterolemia, dyslipidemia without familial hypercholesterolemia and healthy controls.  
*Teodoro Bottiglieri, Baylor Scott & White Research Institute, United States* | 364 |
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Abstract #</th>
</tr>
</thead>
</table>
| 3:30 p.m. – 5 p.m. | **Session 11. Vendor Session**  
(Presented by Platinum and Gold Sponsors)  
*Session Chair: Oscar Yanes* | Auditorium 2 |
| 3:30 p.m. – 4:15 p.m. | **PLATINUM PRESENTERS** –  
SCIEX: Jean-Baptiste Vincendet, Life Sciences Research Market Development, France  
Thermo Fisher Scientific: Susan S. Bird, Sr. Manager, Metabolomics Marketing, USA  
Bruker:  
Agilent Technologies, Inc: Genevieve Van de Bittner, R&D Researcher, USA |            |
| 4:15 p.m. – 5:00 p.m. | **GOLD PRESENTERS** –  
LECO Corporation: David E. Alonso, Applications Chemist, USA  
Metware Biotechnology: Jeffrey Chu, General Manager, North America, USA  
Shimadzu Europa GmbH: Emily Armitage, Research Scientist, UK  
Biocrates Life Sciences AG: Alice Limonciel, Senior Scientist |            |
| 3:30 p.m. – 5 p.m. | **Session 12. Plant and Environmental Applications I**  
*Session Chairs: Maria Pilar Lopez Gresa and Gerhard Prinsloo* | Multi Purpose 1 |
| 3:30 p.m. – 3:50 p.m. | 12.1  
Extending metabolome coverage through a multi-platform approach: the effect of low-dose polychlorinated biphenyls on pig metabolism  
*Luca Narduzzi, University Of Granada, Spain* | 170 |
| 3:50 p.m. – 4:05 p.m. | 12.2  
Computational metabolomics tools reveal metabolic reconfigurations underlying the effects of biostimulant seaweed extracts on maize plants under drought stress conditions  
*Morena Tinte, University Of Johannesburg, South Africa* | 181 |
| 4:05 p.m. – 4:25 p.m. | 12.3  
The Livestock Metabolome Database: application of metabolomics in livestock research  
*Seyed Ali Goldansaz, University Of Alberta, Canada* | 314 |
| 4:25 p.m. – 4:40 p.m. | 12.4  
Leaf metabolomic changes of temperate and tropical seagrass species under future climate change  
*Maria Jung, The University of Western Australia, Australia* | 118 |
| 4:40 p.m. – 5 p.m. | 12.5  
Development of Rapid Evaporative Ionisation Mass Spectrometry (REIMS) for in situ Metabolomics of Plants and Seeds  
*Alice Flint, Queen’s University Belfast, United Kingdom* | 266 |
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Abstract #</th>
</tr>
</thead>
</table>
| 8:30 a.m. – 9:30 a.m. | **Plenary Session 3**  
Ultra-Resolution Plant Metabolomics: High Confidence Metabolite Identification and  
Spatial Analysis at the Cell Type and Organelle Level  
Asaph Aharoni, Weizmann Institute of Science, Israel | Auditorium 1 |
| 10:15 a.m. – 12 noon | **Session 13. Cancer**  
**Session Chairs: Agustín Lahoz Rodríguez and Laimdota Zizmare** | Auditorium 1 |
| 10:15 a.m. – 10:45 a.m. | **13.1 SESSION KEYNOTE**  
The metabolomic way for the screening of endometrial cancer  
Jacopo Troisi, Theoreo srl – spinoff company of the University of Salerno, Italy | 112 |
| 10:45 a.m. – 11:05 a.m. | **13.2**  
Longitudinal modelling reveals distinct changes in circulating metabolites and  
lipoprotein subfractions after breast cancer treatment  
Guro F. Giskeødegård, Norwegian University of Science and Technology, Norway | 182 |
| 11:05 a.m. – 11:20 a.m. | **13.3**  
Discovery and validation of a pre-diagnostic metabolic marker of glioma  
Sebastian Jonsson, Department of Chemistry, Umeå University, Sweden | 196 |
| 11:20 a.m. – 11:40 a.m. | **13.4**  
From features to function: Combining new metabolomics methods to study disease  
and treatment mechanisms in cancer cells  
James Mccullagh, University Of Oxford, United Kingdom | 325 |
| 11:40 a.m. – 11:55 a.m. | **13.5**  
Stable Isotope tracing uncovers global metabolic reprogramming and candidate cancer  
susceptibility pathways in Fanconi Anemia  
Sara Vicente-Muñoz, Cincinnati Children’s Hospital Medical Center, United States | 147 |
| 10:15 a.m. – 12 noon | **Session 14. Collaborative Data Science & Cloud Computing**  
**Session Chairs: Fabien Jourdan and Vinicius Veri** | Auditorium 2 |
| 10:15 a.m. – 10:45 a.m. | **14.1 SESSION KEYNOTE**  
GNPS Dashboard: collaborative exploration of mass spectrometry data in the web browser  
Mingxun Wang, UC San Diego, United States | 237 |
| 10:45 a.m. – 11:05 a.m. | **14.2**  
MZmine 3 – a tool from and for the mass spectrometry community  
Tomáš Pluskal, Institute Of Organic Chemistry And Biochemistry Of The Czech Academy Of Sciences, Czech Republic | 83 |
| 11:05 a.m. – 11:20 a.m. | **14.3**  
CloMet: A novel cloud-based platform that connects established metabolomics data  
repositories and data analysis platforms.  
Roger Mallol, La Salle – Universitat Ramon Llull, Spain | 300 |
| 11:20 a.m. – 11:40 a.m. | **14.4**  
RaMP 2.0 and MetaboSPAN: a public framework for extracting biological and chemical  
insight from metabolomic and multi-omic data  
Ewy Mathe, National Center For Advancing Translational Sciences, United States | 262 |
| 11:40 a.m. – 11:55 a.m. | **14.5**  
FORVM: a Knowledge Graph to decipher associations between metabolites and diseases  
Maxime Delmas, INRAE UMR 1331 ToxAlim, France | 101 |
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Abstract #</th>
</tr>
</thead>
<tbody>
<tr>
<td>10:15 a.m. – 12 noon</td>
<td><strong>Session 15. Technology Advancements II</strong>&lt;br&gt;Session Chairs: Roy Goodacre and Dimitrios Damalas</td>
<td>Multi Purpose 1</td>
</tr>
<tr>
<td>10:15 a.m. – 10:45 a.m.</td>
<td><strong>15.1 KEYNOTE</strong>&lt;br&gt;Next Gen Metabolomics Technologies: Deeper Coverage, Single Cell, Double Bond Pinpointing, Ion Mobility and Imaging&lt;br&gt;Facundo Fernandez, Georgia Institute Of Technology, United States</td>
<td>389</td>
</tr>
<tr>
<td>10:45 a.m. – 11:05 a.m.</td>
<td><strong>15.2</strong>&lt;br&gt;Breath analysis by secondary electrospray high-resolution mass spectrometry: An interoperability framework for multicentric studies and metabolic phenotyping&lt;br&gt;Kapil Dev Singh, University of Basel, Switzerland</td>
<td>138</td>
</tr>
<tr>
<td>11:05 a.m. – 11:20 a.m.</td>
<td><strong>15.3</strong>&lt;br&gt;A universal ion mobility calibration for interoperable collision cross section databases&lt;br&gt;Anaïs George, Laboratoire COBRA, France</td>
<td>45</td>
</tr>
<tr>
<td>11:20 a.m. – 11:40 a.m.</td>
<td><strong>15.4</strong>&lt;br&gt;Mapping the metabolome of living cells using Laser Desorption-Rapid Evaporative Ionization Mass Spectrometry (LD-REIMS)&lt;br&gt;Stefania Maneta-Stavrakaki, Imperial College London, United Kingdom</td>
<td>322</td>
</tr>
<tr>
<td>11:40 a.m. – 11:55 a.m.</td>
<td><strong>15.5</strong>&lt;br&gt;Ion Mobility Mass Spectrometry for the Characterization of Urolithin Glucuronides&lt;br&gt;Maria Moran-Garrido, Centro de Metabolómica y Bioanálisis (CEMBIO), Facultad de Farmacia, Universidad San Pablo-CEU, CEU Universities, Spain</td>
<td>225</td>
</tr>
<tr>
<td>12:20 p.m. – 1:20 p.m.</td>
<td><strong>Sponsor Lunch Presentations</strong></td>
<td></td>
</tr>
</tbody>
</table>
## Wednesday, June 22

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Abstract #</th>
</tr>
</thead>
</table>
| 1:30 p.m. – 3 p.m. | Session 16. Lung and Respiratory Diseases  
*Session Chairs: Craig Wheelock and Julia Kuligowski* | Auditorium 1 |
| 1:30 p.m. – 1:50 p.m. | 16.1 MiR-342-3p and immune mediated metabolic signatures as drivers of long-term lung trajectories  
Sofina Begum, Brigham And Women's Hospital, Harvard Medical School, United States | 296         |
| 1:50 p.m. – 2:05 p.m. | 16.2 Non-Invasive Prediction of Oxidative Stress and Inflammation Markers in Children by Exhaled Breath Metabolites  
Amanda Gisler, University Children's Hospital Basel UKBB, University Of Basel, Switzerland, Switzerland | 63          |
| 2:05 p.m. – 2:25 p.m. | 16.3 GC-MS profiling of volatile metabolites produced by bacteria causing Ventilation-Associated Pneumonia  
Wojciech Filipiak, Dept of Pharmacodynamics and Molecular Pharmacology, Collegium Medicum UMK, Poland | 306         |
| 2:25 p.m. – 2:40 p.m. | 16.4 Benchtop Nuclear Magnetic Resonance-based metabolomic approach for the diagnosis of tuberculosis  
Jose Luis Izquierdo García, UCM, España | 332         |
| 2:40 p.m. – 3 p.m. | 16.5 Multi-omic landscape of squamous cell lung cancer  
Paul Stewart, Moffitt Cancer Center, United States | 109         |

| 1:30 p.m. – 3 p.m. | Session 17. Plant and Environmental Applications II  
*Session Chairs: Ian Dubery and Antonio Granell* | Auditorium 2 |
| 1:30 p.m. – 1:50 p.m. | 17.1 Metabolomics applications in plant sciences: elucidating mode of actions of biostimulants  
Fidele Tugizimana, University Of Johannesburg & Omnia Group Ltd, South Africa | 231         |
| 1:50 p.m. – 2:05 p.m. | 17.2 1HNMR-based metabolomics analysis as a tool to identify antiviral compounds from unrelated plants  
Gerhard Prinsloo, University Of South Africa, South Africa | 54          |
| 2:05 p.m. – 2:25 p.m. | 17.3 Utility of Metabolomics to Support Read-Across and Category Justification for UVCB substances in REACH  
Hennicke Kamp, Basf Metabolome Solutions Gmbh, Germany | 299         |
| 2:25 p.m. – 2:40 p.m. | 17.4 Gut metabolomics after the exposure to diclofenac and selenium supplementation  
Gema Moro, University Of Huelva, Spain | 133         |
| 2:40 p.m. – 3 p.m. | 17.5 Coupling growth of Pseudomonas putida to a synthetic fluorination metabolism  
Corey Griffith, Luxembourg Centre for Systems Biomedicine, Luxembourg | 187         |
### Wednesday, June 22

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Abstract #</th>
</tr>
</thead>
<tbody>
<tr>
<td>1:30 p.m. – 3 p.m.</td>
<td><strong>Session 18. QA/QC and Reproducibility</strong>&lt;br&gt;<strong>Session Chairs: Tracey Schock and Michael Witting</strong></td>
<td>Multi Purpose 1</td>
</tr>
<tr>
<td>1:30 p.m. – 1:50 p.m.</td>
<td>18.1 mQACC: A community-led initiative to strengthen quality assurance and quality control practices and reporting in untargeted metabolomics research&lt;br&gt;<em>Matthew Lewis, Bruker Life Sciences, United Kingdom</em></td>
<td>110</td>
</tr>
<tr>
<td>1:50 p.m. – 2:05 p.m.</td>
<td>18.2 Reporting Standards: How to ensure everyone else knows your metabolomics data is good quality&lt;br&gt;<em>Jennifer Kirwan, Berlin Institute Of Health At Charite, Germany</em></td>
<td>205</td>
</tr>
<tr>
<td>2:05 p.m. – 2:25 p.m.</td>
<td>18.3 Long-term storage has minor effects on biobanked neonatal dried blood spot metabolome&lt;br&gt;<em>Filip Ottosson, Statens Serum Institut, Denmark</em></td>
<td>242</td>
</tr>
<tr>
<td>2:25 p.m. – 2:40 p.m.</td>
<td>18.4 Interlaboratory comparison of metabolomics analyses of human and rodent blood using Biocrates MxP® Quant 500 kit&lt;br&gt;<em>Gabi Kastenmüller, Helmholtz Zentrum München, Germany</em></td>
<td>128</td>
</tr>
<tr>
<td>2:40 p.m. – 3 p.m.</td>
<td>18.5 Hemoglobin normalization outperforms other methods for standardizing dried blood spot metabolomics: A comparative study&lt;br&gt;<em>Abhishek Jain, Yale University, United States</em></td>
<td>157</td>
</tr>
<tr>
<td>3:30 p.m. – 5 p.m.</td>
<td><strong>Session 19. Metabolomics Throughout the Lifecourse</strong>&lt;br&gt;<strong>Session Chairs: Lorraine Brennan and Evelina Charidemou</strong></td>
<td>Auditorium 1</td>
</tr>
<tr>
<td>3:30 p.m. – 3:50 p.m.</td>
<td>19.1 Steroids play distinct roles in pregnancy compared to early life for childhood infection proneness&lt;br&gt;<em>Nicole Prince, Harvard Medical School, Brigham and Women’s Hospital, United States</em></td>
<td>146</td>
</tr>
<tr>
<td>3:50 p.m. – 4:05 p.m.</td>
<td>19.2 Struggling to make it to the egg: metabolomics of seminal liquid to understand human fertility decline&lt;br&gt;<em>Víctor González-ruiz, University Of Geneva, Switzerland</em></td>
<td>272</td>
</tr>
<tr>
<td>4:05 p.m. – 4:25 p.m.</td>
<td>19.3 Lipidomic profiling of extracellular vesicles derived from human milk samples&lt;br&gt;<em>Isabel Ten-Doménech, Health Research Institute La Fe, Spain</em></td>
<td>161</td>
</tr>
<tr>
<td>4:25 p.m. – 4:40 p.m.</td>
<td>19.4 Connectivity between phosphatidylcholine biosynthesis, aging and energy metabolism unravelled by NMR-based metabolomics&lt;br&gt;<em>Qishun Zhou, Medical University of Graz, Austria</em></td>
<td>260</td>
</tr>
<tr>
<td>4:40 p.m. – 5 p.m.</td>
<td>19.5 Translating biological models of the ageing metabolome in to clinically relevant biomarkers.&lt;br&gt;<em>Nicholas Rattray, University of Strathclyde, United Kingdom</em></td>
<td>224</td>
</tr>
</tbody>
</table>
### Wednesday, June 22

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Abstract #</th>
</tr>
</thead>
</table>
| **3:30 p.m. – 5 p.m.** | Session 20. Met ID II  
*Session Chairs: Justin JJ Van der Hooft and* | Auditorium 2 |
| 3:30 p.m. – 3:50 p.m. | **20.1** Improving reliability of small molecule identification using spectral entropy and retention time prediction  
*Sajjan Mehta, oloBion, Spain* | 189 |
| 3:50 p.m. – 4:05 p.m. | **20.2** CPExtract, a novel software tool for the comprehensive detection of tracer-derived metabolites in high resolution mass spectrometry data  
*Bernhard Seidl, Institute for Bioanalytics and Agro-Metabolomics, IFA-Tulln, University of Natural Resources and Life Sciences, Austria* | 236 |
| 4:05 p.m. – 4:25 p.m. | **20.3** Ion Identity Molecular Networking for Mass Spectrometry-based Metabolomics  
*Robin Schmid, Skaggs School of Pharmacy, University of California San Diego, Vereinigte Staaten* | 239 |
| 4:25 p.m. – 4:40 p.m. | **20.4** Multi-network integration to analyze non-targeted LC-MS metabolomics data from Caenorhabditis elegans  
*Liesa Salzer, Helmholtz Zentrum Muenchen, Germany* | 51 |
| 4:40 p.m. – 5 p.m. | **20.5** CMM 4.0: improving the metabolite annotation using RT and CCS prediction  
*Alberto Gil-de-la-fuente, CEU-San Pablo University, Spain* | 234 |
| **3:30 p.m. – 5 p.m.** | Session 21. Metabolic Diseases  
*Session Chairs: Rachel Kelly and Natasa Giallourou* | Multi Purpose 1 |
| 3:30 p.m. – 3:50 p.m. | **21.1** Lipidomic profile of white adipose tissue associated with obesity and insulin resistance in pregnant women with previous bariatric surgery  
*Susana Alejandra Palma Duran, The Francis Crick Institute, United Kingdom* | 337 |
| 3:50 p.m. – 4:05 p.m. | **21.2** UHPLC-MS/MS-based Metabolomics reveals differences on Extracellular Vesicles secreted by obese hepatocytes, and their effects on adipocyte metabolism  
*Maria Azparren-Angulo, Cicbiogune, Spain* | 154 |
| 4:05 p.m. – 4:25 p.m. | **21.3** Low carbohydrate high fat diet improves composition of the circulating lipids in people with type 2 diabetes  
*Kajetan Trošt, University of Copenhagen, Denmark* | 92 |
| 4:25 p.m. – 4:40 p.m. | **21.4** Plasma metabolic profile of subclinical atherosclerosis in South-East Asians.  
*Nilanjana Sadhu, Nanyang Technological University Lee Kong Chian School of Medicine, Singapore* | 193 |
| 4:40 p.m. – 5 p.m. | **21.5** NAD+ – an old cofactor with new tricks  
*Sofia Moco, VU Amsterdam, Netherlands* | 312 |
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Abstract #</th>
</tr>
</thead>
</table>
| 8:30 a.m. – 10:15 a.m. | **Session 22. Microbiome and Gastrointestinal Function**  
*Session Chairs: Daniel Raftery and Maria Eugenia Monge* | Auditorium 1 |
| 8:30 a.m. – 9:00 a.m. | **22.1 SESSION KEYNOTE** Spacial-, temporal- and inter-person variation of metabolites across the upper and lower human gastrointestinal tract.  
*Oliver Fiehn, UC Davis, United States* | 253 |
| 9:00 a.m. – 9:20 a.m. | **22.2** Quantitative Sensitive CHEmoselective Metabolomics Analysis (Quant-SCHEMA) – Detailed investigation of microbiome metabolism  
*Daniel Globisch, Uppsala University, Sweden* | 228 |
| 9:20 a.m. – 9:35 a.m. | **22.3** Chemical exposures are associated with altered microbiome and secondary bile acid pathways in obesity and insulin resistance  
*Partho Sarathi Sen, Turku Bioscience, University Of Turku, Finland* | 186 |
| 9:35 a.m. – 9:55 a.m. | **22.4** Gut microbiome-linked metabolites in the pathobiology of depression and anxiety – a role for bile acids  
*Rima Kaddurah-Daouk, Duke University Medical Center, United States* | 359 |
| 9:55 a.m. – 10:10 a.m. | **22.5** Metabolome Alterations in a Mouse Model Support Microbiome-Metabolite Interactions in a Cohort of Children With Cow’s Milk Allergy  
*Ellen De Paepe, Ghent University, Belgium* | 165 |
| 8:30 a.m. – 10:15 a.m. | **Session 23. Natural Products**  
*Session Chairs: Fidele Tugizimana and Maria Garcia Altares* | Auditorium 2 |
| 8:30 a.m. – 9:00 a.m. | **23.1 SESSION KEYNOTE** Helichrysum umbraculigerum: A new plant system for cannabinoid biochemistry  
*Paula Berman, Weizmann Institute of Science, Israel* | 315 |
| 9:00 a.m. – 9:20 a.m. | **23.2** Unraveling 100 plant glycosyltransferases with 600 Natural compounds: results of a combinatorial screen  
*Elys Rodriguez, Fiehn Lab, United States* | 257 |
| 9:20 a.m. – 9:35 a.m. | **23.3** Deciphering the Complex Chemical Space and Biosynthetic Routes of Steroidal Saponins in Monocotyledonous Plants  
*Adam Jozwiak, Weizmann Institute of Science, Israel* | 318 |
| 9:35 a.m. – 9:55 a.m. | **23.4** Identification of natural products as potential plant-derived herbicides through metabolomics  
*Monica Scognamiglio, University Of Campania “Luigi Vanvitelli”, DiSTABiF, Italy* | 316 |
| 9:55 a.m. – 10:10 a.m. | **23.5** Exploiting metabolic diversity in Nicotiana for intragenic production of squalene  
*Margit Drapal, Royal Holloway University Of London, United Kingdom* | 177 |
**Thursday, June 23**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Abstract #</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:30 a.m. – 10:15 a.m.</td>
<td><strong>Session 24. Analytical Methods in Lipidomics</strong>&lt;br&gt;<strong>Session Chairs: Matej Oresic and Susana Palma</strong></td>
<td>Multi Purpose 1</td>
</tr>
<tr>
<td>8:30 a.m. – 9:00 a.m.</td>
<td><strong>24.1 KEYNOTE</strong>&lt;br&gt;Lipidomics and epilipidomics signature of human obesity and insulin resistance&lt;br&gt;<strong>Maria Fedorova, Technical University Dresden, Germany</strong></td>
<td>454</td>
</tr>
<tr>
<td>9:00 a.m. – 9:20 a.m.</td>
<td><strong>24.2</strong>&lt;br&gt;Metabolic profiling of octadecanoid oxylipins using chiral supercritical fluid chromatography coupled to tandem mass spectrometry&lt;br&gt;<strong>Craig Wheelock, Karolinska Institute, Sweden</strong></td>
<td>292</td>
</tr>
<tr>
<td>9:20 a.m. – 9:35 a.m.</td>
<td><strong>24.3</strong>&lt;br&gt;High-throughput Plasma Lipidomics using Ion-mobility enhanced DDA and DIA Mass Spectrometry (DDA-PASEF/diaPASEF)&lt;br&gt;<strong>Premy Shanthamoorthy, University of Toronto, Canada</strong></td>
<td>66</td>
</tr>
<tr>
<td>9:35 a.m. – 9:55 a.m.</td>
<td><strong>24.4</strong>&lt;br&gt;Complete structure elucidation of lipids by electron activated dissociation mass spectrometry&lt;br&gt;<strong>Takashi Baba, Sciex, Canada</strong></td>
<td>134</td>
</tr>
<tr>
<td>9:55 a.m. – 10:10 a.m.</td>
<td><strong>24.5</strong>&lt;br&gt;Ultra-high throughput metabolomics and lipidomics: Results from the first 5,000 samples&lt;br&gt;<strong>Zach Rabow, UC Davis, United States</strong></td>
<td>350</td>
</tr>
<tr>
<td>11:30 a.m. – 1 p.m.</td>
<td><strong>Plenary Session 4 and Awards / Closing</strong>&lt;br&gt;Analytical Challenges in Untargeted Metabolomics Workflow&lt;br&gt;<strong>Coral Barbas, Universidad San Pablo CEU, Spain</strong></td>
<td>Auditorium 1</td>
</tr>
<tr>
<td>1 p.m.</td>
<td><strong>Boxed Lunch to Go</strong></td>
<td></td>
</tr>
</tbody>
</table>