



# METABOLOMICS2025

PRAGUE, CZECH REPUBLIC

JUNE 22-26

21<sup>st</sup> Annual Conference of the Metabolomics Society



SCHEDULE OF  
**ORAL PRESENTATIONS**

# AGENDA AT A GLANCE

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

## SUNDAY, JUNE 22

|                        | North Hall  | South Hall 1                                     | South Hall 2                       |
|------------------------|---|--|------------------------------------|
| 11:00 a.m.             | <b>REGISTRATION OPEN</b>                              |  |                                    |
| 12:00 p.m. – 2:00 p.m. | <b>W1: Part 1</b> Web-based Tools for Microbiome Data | <b>W2:</b> Metabolome Xchange                    |                                    |
| 2:15 p.m. – 4:15 p.m.  | <b>W1: Part 2</b> Web-based Tools for Microbiome Data | <b>W3:</b> Reverse Met Big Data Discovery        | <b>W4:</b> Volatilomics            |
| 4:30 p.m. – 6:30 p.m.  | <b>W5:</b> mzmine Data Analysis                       | <b>W6:</b> Demystifying Stable Isotope Labelling | <b>W7:</b> Clinical Implementation |
| 6:45 p.m. – 8:00 p.m.  | <b>Career Night – Roundtable Discussions</b>          |  |                                    |

## MONDAY, JUNE 23

|                         | North Hall  | South Hall 1                                   | South Hall 2                            |
|-------------------------|---|--|---|
| 7:30 a.m.               | <b>REGISTRATION / INFO DESK OPEN</b>  |  |   |
| 8:15 a.m. – 10:15 a.m.  | <b>W8:</b> Mass Spectra MS2LDA  | <b>W9:</b> Met Data Standard for AI            | <b>W10:</b> EMN Metabo Mentors          |
| 10:15 a.m. – 10:30 a.m. | <b>BREAK</b>  |  |   |
| 10:30 a.m. – 12:30 p.m. | <b>W11:</b> Automated Annotation SIRIUS 6                                   | <b>W12:</b> Beyond CID Met/Lipid ID            | <b>W13:</b> Best Practices MQACC        |
| 12:30 p.m. – 1:30 p.m.  | <b>LUNCH BREAK (on your own)</b>  |  |   |
| 1:30 p.m. – 3:00 p.m.   | <b>Opening Ceremony &amp; Plenary Session 1</b> – Livia Schiavinato Eberlin |  |   |
| 3:00 p.m. – 3:30 p.m.   | <b>BREAK</b>  |  |   |
|                         | <b>Congress Hall</b>  | <b>South Hall 1</b>                            | <b>South Hall 2</b>                     |
| 3:30 p.m. – 5:15 p.m.   | <b>1</b> Cellular Metabolism  | <b>2</b> Predictive Approaches and Simulations | <b>3</b> New Avenues for Lipid Analysis |
| 5:15 p.m. – 6:45 p.m.   | <b>Welcome Reception – Poster Session 1</b>                                 |  |   |
| 7:00 p.m. – 8:00 p.m.   | <b>Metabolomics Society Town Hall Meeting</b>                               |  |   |

## TUESDAY, JUNE 24

|                         | Congress Hall   | South Hall 1   | South Hall 2                                   |
|-------------------------|---|--|--|
| 7:45 a.m.               | <b>REGISTRATION / INFO DESK OPEN</b>                          |  |  |
| 8:30 a.m. – 9:30 a.m.   | <b>Plenary Session 2</b> – Erin Baker                         |  |  |
| 9:30 a.m. – 10:15 a.m.  | <b>BREAK</b>  |  |  |
| 9:40 a.m. – 10:10 a.m.  | <b>BioHub 1:</b> CcpNmr Analysis Metabolomics                 |  |  |
| 9:45 a.m. – 10:00 a.m.  | <b>Exhibitor Demo Pres:</b> Beckman Coulter for Life Sciences |  |  |
| 10:15 a.m. – 12:00 p.m. | <b>4</b> Clinical Translation of Lipidomics & Met             | <b>5</b> Quantitative and Statistical Methods        | <b>6</b> Natural Product Discovery from Plants |
| 12:00 p.m. – 1:30 p.m.  | <b>LUNCH BREAK AND SPONSOR PRESENTATIONS</b>                  |  |  |
| 12:20 p.m. – 1:20 p.m.  | <b>Sponsor Pres:</b> Thermo Fisher Scientific                 |  | <b>Sponsor Pres:</b> SCIEX                     |
| 1:30 p.m. – 3:00 p.m.   | <b>7</b> Data Repositories and Curation                       | <b>8</b> Mass Spectrometry Imaging                   | <b>9</b> Microbial Metabolomics                |
| 3:00 p.m. – 3:30 p.m.   | <b>BREAK</b>  |  |  |
| 3:00 p.m. – 3:25 p.m.   | <b>BioHub 2:</b> Metabonaut: LC-MS/MS                         |  |  |
| 3:30 p.m. – 5:15 p.m.   | <b>10</b> Vendor Session                                      | <b>11</b> Pregnancy, Neonatal, Early Life Metabolism | <b>12</b> Agricultural and Animal Products     |
| 5:15 p.m. – 6:45 p.m.   | <b>Poster Session 2</b>                                       |  |  |
| 6:45 p.m. – 8:15 p.m.   | <b>EMN Reception</b>  |  |  |

## WEDNESDAY, JUNE 25

|                         | Congress Hall  | South Hall 1   | South Hall 2   |
|-------------------------|--|--|--|
| 8:00 a.m.               | <b>REGISTRATION / INFO DESK OPEN</b>                 |  |  |
| 8:30 a.m. – 9:30 a.m.   | <b>Plenary Session 3</b> – Steffen Neumann           |  |  |
| 9:30 a.m. – 10:15 a.m.  | <b>BREAK</b>   |  |  |
| 9:40 a.m. – 10:10 a.m.  | <b>BioHub 3:</b> Using PARADISE                      |  |  |
| 9:45 a.m. – 10:00 a.m.  | <b>Exhibitor Demo Pres:</b> Metabolon                |  |  |
| 10:15 a.m. – 12:00 p.m. | <b>13</b> Multi-omics and Integrative Methods        | <b>14</b> Microbiome and Host-Metabolism Interactions  | <b>15</b> Natural Products and Plant Defense         |
| 12:00 p.m. – 1:30 p.m.  | <b>LUNCH BREAK AND SPONSOR PRESENTATIONS</b>         |  |  |
| 12:20 p.m. – 1:20 p.m.  | <b>Sponsor Pres:</b> Waters                          |  | <b>Sponsor Pres:</b> Bruker                          |
| 1:30 p.m. – 3:00 p.m.   | <b>16</b> Age-Related Diseases and Cancer            | <b>17</b> Biomonitoring and Environmental Metabolomics | <b>18</b> Metabolomics Beyond LC-MS: NMR and More    |
| 3:00 p.m. – 3:30 p.m.   | <b>BREAK</b>   |  |  |
| 3:00 p.m. – 3:25 p.m.   | <b>BioHub 4:</b> Metabox 2.0 and SiMD                |  |  |
| 3:10 p.m. – 3:25 p.m.   | <b>Exhibitor Demo Pres:</b> Thermo Fisher Scientific |  |  |
| 3:30 p.m. – 5:15 p.m.   | <b>19</b> Metabolite Annotation                      | <b>20</b> Cardiovascular & Endocrine Disease           | <b>21</b> Going Small – Low Volume and Sample Amount |
| 5:15 p.m. – 6:45 p.m.   | <b>Poster Session 3</b>                              |  |  |
| 7:30 p.m. – 10:30 p.m.  | <b>Conference Dinner</b>                             |  |  |

## THURSDAY, JUNE 26

|                         | Congress Hall  | South Hall 1                               | South Hall 2                                  |
|-------------------------|--|--|---|
| 8:15 a.m.               | <b>REGISTRATION / INFO DESK OPEN</b>                               |  |   |
| 8:30 a.m. – 9:30 a.m.   | <b>Plenary Session 4</b> – Peter Meikle                            |  |   |
| 9:30 a.m. – 10:30 a.m.  | <b>Poster Session 4</b>  |  |   |
| 9:40 a.m. – 10:10 a.m.  | <b>BioHub 5:</b> MSlineAR Software                                 |  |   |
| 10:30 a.m. – 12:15 p.m. | <b>22</b> Nutrition and Exosome Research                           | <b>23</b> Food, Health, and Sustainability | <b>24</b> Data Processing and Cheminformatics |
| 12:15 p.m. – 1:30 p.m.  | <b>LUNCH BREAK AND SPONSOR PRESENTATIONS</b>                       |  |   |
| 12:25 p.m. – 1:25 p.m.  |  |  | <b>Sponsor Pres:</b> Agilent                  |
| 1:30 p.m. – 3:15 p.m.   | <b>Plenary Session 5</b> – Clary Clish – <b>Awards and Closing</b> |  |   |

★ **AWARD WINNERS**

| Monday, June 23       |  |                      |
|-----------------------|--|----------------------|
| Time                  | Session  | Abstract #           |
| 1:30 p.m. – 3:00 p.m. | <b>Opening Ceremony &amp; Plenary Session 1</b><br><i>Livia Schiavinato Eberlin, Baylor College Of Medicine, United States</i><br>Guiding Clinical Decisions with Metabolic information provided by Direct Mass Spectrometry Analysis              | <i>Congress Hall</i> |
| 3:30 p.m. – 5:15 p.m. | <b>Session 1. Cellular Metabolism</b><br><i>Session Chairs: Howbeer Muhamadali and Ellen De Paepe</i>  | <i>Congress Hall</i> |
| 3:30 p.m. – 4:00 p.m. | <b>1.1 KEYNOTE</b><br>Hyperacetylated histone H4 is a source of carbon contributing to lipid synthesis<br><i>Evelina Charidemou, University Of Nicosia, Cyprus</i>   | <b>168</b>           |
| 4:00 p.m. – 4:20 p.m. | <b>1.2</b><br>Uncovering mechanisms of thiazolidinediones on osteogenesis and adipogenesis using spatial fluxomics<br><i>Ondrej Kuda, Institute Of Physiology, Czech Academy Of Sciences, Czech Republic</i>                                       | <b>179</b>           |
| 4:20 p.m. – 4:40 p.m. | <b>1.3</b><br>Lipidomics, metabolomics and <sup>13</sup> C glucose tracing reveal the effects of hyperinsulinemia in sucrose-induced insulin resistance<br>★ <i>Haoning Howard Cen, Life Sciences Inst, University of British Columbia, Canada</i> | <b>493</b>           |
| 4:40 p.m. – 5:00 p.m. | <b>1.4</b><br>Metabolic Reprogramming Drives Immunometabolic and Neuroinflammatory Dysregulation in Treated HIV<br><i>Ujjwal Neogi, Karolinska Institutet, Sweden</i>  | <b>328</b>           |
| 5:00 p.m. – 5:15 p.m. | <b>1.5</b><br>Space Metabolomics: Investigating Neural Stem Cell Adaptations to Microgravity<br>★ <i>Lucie Davidová, Uppsala University, Sweden</i>  | <b>180</b>           |
| 3:30 p.m. – 5:15 p.m. | <b>Session 2. Predictive Approaches and Simulations</b><br><i>Session Chairs: Sebastian Böcker and Rasmus Bro</i>  | <i>South Hall 1</i>  |
| 3:30 p.m. – 4:00 p.m. | <b>2.1 KEYNOTE</b><br>Simulated metabolic profiles reveal biases in pathway analysis methods<br><i>Fabien Jourdan, INRAE-MetaboHUB, France</i>   | <b>546</b>           |
| 4:00 p.m. – 4:20 p.m. | <b>2.2</b><br>Topology-Aware Single Sample Pathway Analysis using the Graph Fourier Transform<br><i>Tom Rix, Imperial College London, United Kingdom</i>   | <b>390</b>           |
| 4:20 p.m. – 4:40 p.m. | <b>2.3</b><br>Data-driven <sup>13</sup> C-fluxomics towards ab initio reconstruction of metabolic networks.<br><i>Noémie Butin, MetaboHub-MetaToul, France</i>   | <b>377</b>           |
| 4:40 p.m. – 5:00 p.m. | <b>2.4</b><br>Times are changing but order matters: Transferable prediction of small molecule liquid chromatography retention times<br><i>Fleming Kretschmer, Friedrich Schiller University Jena, Germany</i>                                      | <b>170</b>           |
| 5:00 p.m. – 5:15 p.m. | <b>2.5</b><br>Bridging polarities in metabolomics: Cross-ionization mode chemical similarity prediction between tandem mass spectra<br>★ <i>Niek de Jonge, Wageningen Univ. &amp; Res., Netherlands</i>  | <b>31</b>            |

## ★ AWARD WINNERS

| Monday, June 23              |   |                     |
|------------------------------|---|---------------------|
| Time                         | Session   | Abstract #          |
| <b>3:30 p.m. – 5:15 p.m.</b> | <b>Session 3. New Avenues for Lipid Analysis</b><br><i>Session Chairs: Peter Meikle and Alex Dickens</i>  | <b>South Hall 2</b> |
| 3:30 p.m. – 4:00 p.m.        | <b>3.1 KEYNOTE</b><br>ZT Scan DIA with Two-Dimensional Deconvolutions for Untargeted Metabolomics<br>★ <i>Hiroshi Tsugawa, TUAT, Japan</i>  | <b>193</b>          |
| 4:00 p.m. – 4:20 p.m.        | <b>3.2</b><br>Expanding the Annotation of Esterified Oxylipins Using Multidimensional Databases and LC-MS/MS-based Ion Identity Molecular Networking Analysis<br><i>Sandra M. Camunas-Alberca, Centro de Metabolómica y Bioanálisis (CEMBIO), Spain</i> | <b>315</b>          |
| 4:20 p.m. – 4:40 p.m.        | <b>3.3</b><br>A metabolite array for 10-second classification of brain cancers with ambient mass spectrometry: towards a pilot database using 1,300 patients<br><i>Arash Zarrine-Afsar, University of Toronto, Canada</i>                               | <b>58</b>           |
| 4:40 p.m. – 5:00 p.m.        | <b>3.4</b><br>Innovations in Skin Ceramide Profiling: Leveraging Supercritical Fluid Chromatography and High-Resolution Mass Spectrometry (Q-ToF) for Advanced Analysis<br><i>Justine Bertrand-Michel, MetaboHUB-metatoul, France</i>                   | <b>152</b>          |
| 5:00 p.m. – 5:15 p.m.        | <b>3.5</b><br>Development of a Novel High-Throughput Acoustic Droplet Ejection Mass Spectrometry Method with Signal Durations for Lipidomics<br><i>Yu Zhang, Leiden University, Netherlands</i>   | <b>127</b>          |

## Tuesday, June 24


| Time                    | Session  | Abstract #           |
|-------------------------|--|----------------------|
| 8:30 a.m. – 9:30 a.m.   | <b>Plenary Session 2</b><br><i>Erin Baker, University of North Carolina at Chapel Hill, United States</i><br>You Are What You Breathe and Eat: Linking Chemical Exposure and Molecular Responses                     | <b>Congress Hall</b> |
| 9:30 a.m. – 10:15 a.m.  | <b>BREAK</b>   |                      |
| 9:40 a.m. – 10:10 a.m.  | <b>BioHub 1</b><br>Profiling 1D1H NMR metabolomics spectra with the CcpNmr Analysis Metabolomics Software via interactive and semi-automated curve-fitting of curated simulated metabolite standards                 |                      |
| 9:45 a.m. – 10:00 a.m.  | <b>EXHIBITOR DEMO PRESENTATION – GOLD SPONSOR</b><br><b>Beckman Coulter for Life Sciences</b><br>Enhance Your Metabolomics Research With Automated Liquid Handling<br><i>Rene Goedde, Market Development Manager</i> |                      |
|                         |   |                      |
| 10:15 a.m. – 12:00 p.m. | <b>Session 4. Clinical Translation of Lipidomics &amp; Metabolomics</b><br><i>Session Chairs: Jessica Lasky-Su and Nicholas Rattray</i>  | <b>Congress Hall</b> |
| 10:15 a.m. – 10:45 a.m. | <b>4.1 SESSION KEYNOTE</b><br>Comprehensive, quantitative analysis of SRM 1950: the NIST human plasma reference material<br><i>Rupasri Mandal, University Of Alberta, Canada</i>                                     | <b>500</b>           |
| 10:45 a.m. – 11:05 a.m. | <b>4.2</b><br>Bridging the Gap: from Research-Grade Methods to Routine Clinical Applications<br><i>Anne Bendt, National University of Singapore, Singapore</i>   | <b>407</b>           |
| 11:05 a.m. – 11:25 a.m. | <b>4.3</b><br>Pharmacometabolomics reveals notable differences between real-world and expected drug metabolism patterns<br><i>Frank Klont, University Of Groningen, Netherlands</i>                                  | <b>40</b>            |
| 11:25 a.m. – 11:45 a.m. | <b>4.4</b><br>Metabolomics and clinical chemistry insights from 20,000 individuals<br><i>Natasa Giallourou, Metabolon Inc., United States</i>  | <b>273</b>           |
| 11:45 a.m. – 12:00 p.m. | <b>4.5</b><br>Infant formula composition affects tetraglucoside (Glc4) excretion: the impact on the diagnostics of inborn errors of metabolism<br><i>Silvia Radenkovic, UMC Utrecht, Netherlands</i>                 | <b>74</b>            |



★ **AWARD WINNERS**

| Tuesday, June 24               |  |                     |
|--------------------------------|--|---------------------|
| Time                           | Session  | Abstract #          |
| <b>10:15 a.m. – 12:00 p.m.</b> | <b>Session 5. Quantitative and Statistical Methods</b><br><i>Session Chairs: Timothy Ebbels and Roman Bushuiev</i>   | <b>South Hall 1</b> |
| 10:15 a.m. – 10:45 a.m.        | <b>5.1 KEYNOTE</b><br>Overlooked Challenges in Quantitative Metabolomics<br>★ <i>Tao Huan, University of British Columbia, Canada</i>  | <b>520</b>          |
| 10:45 a.m. – 11:05 a.m.        | <b>5.2</b><br>Enhancing biomarker discovery in metabolomics through cooperative learning-based vertical data integration<br>★ <i>Elfried B. M. Salanon, INRAE, France</i>  | <b>400</b>          |
| 11:05 a.m. – 11:25 a.m.        | <b>5.3</b><br>Towards enhanced reproducibility and performance of quality control sample-based normalization: key issues and new ideas<br><i>Matthijs Vynck, Ghent University, Belgium</i>   | <b>427</b>          |
| 11:25 a.m. – 11:45 a.m.        | <b>5.4</b><br>A Bayesian Framework for Integrating Multiple Variable Selection Methods in Metabolomics: A Case study on pneumonia-biomarker detection<br><i>Ioanna Barla, National &amp; Kapodistrian Univ. Of Athens, Greece</i>  | <b>69</b>           |
| 11:45 a.m. – 12:00 p.m.        | <b>5.5</b><br>GcDUO: A Batch Processing Framework Integrating PARAFAC and PARAFAC2 for GC_GC-MS Data Analysis<br>★ <i>Maria Llambrich, Institut d'Investigació Sanitària Pere Virgili (IISPV), Spain</i>                           | <b>414</b>          |
| <b>10:15 a.m. – 12:00 p.m.</b> | <b>Session 6. Natural Product Discovery from Plants</b><br><i>Session Chairs: Norberto Pepporine Lopes and Tito Damiani</i>  | <b>South Hall 2</b> |
| 10:15 a.m. – 10:45 a.m.        | <b>6.1 KEYNOTE</b><br>Integrated Multi-omics Approaches for Discovering Plant Biosynthetic Pathways<br><i>Jing-Ke Weng, Northeastern University, United States</i>   | <b>543</b>          |
| 10:45 a.m. – 11:05 a.m.        | <b>6.2</b><br>Charting the chemical space of South African medicinal plants with computational metabolomics<br><i>Fidele Tugizimana, University Of Johannesburg &amp; Omnia Group Ltd, South Africa</i>                            | <b>402</b>          |
| 11:05 a.m. – 11:25 a.m.        | <b>6.3</b><br>Feature-Based Molecular Networking Guided Discovery and Isolation of Novel Capsaicinoids from the chili pepper ( <i>Capsicum</i> sp.) and their TRPV1 activation<br><i>Joshua Smith, IOCB Prague, Czech Republic</i> | <b>218</b>          |
| 11:25 a.m. – 11:45 a.m.        | <b>6.4</b><br>Integrating Spatial Mapping and Metabolomics: A Novel Platform for Bioactive Discovery and Saline Land Reclamation<br><i>Rossarin Tansawat, Chulalongkorn University, Thailand</i>                                   | <b>405</b>          |
| 11:45 a.m. – 12:00 p.m.        | <b>6.5</b><br>Integrating omics for untargeted discovery of plant specialized metabolites<br>★ <i>Elena Del Pup, Wageningen University &amp; Research, Netherlands</i>   | <b>283</b>          |

## ★ AWARD WINNERS

| Tuesday, June 24  |  |                     |
|---|--|---------------------|
| Time  | Session  | Abstract #          |
| 12:20 p.m. – 1:20 p.m.  | <b>Sponsor Lunch Presentations</b>   |                     |
|  | <b>Thermo Fisher Scientific</b><br>The hardware design and functional impact of the Orbitrap Astral in your metabolomics and lipidomics research<br><i>Alexander Makarov, Sr. Director Global Research, LSMS, Thermo Fisher Scientific</i><br><br>SQUAD on Orbitrap Astral applied to the study of healthy aging lipidome<br><i>Magali Sarafian, Team Lead Metabolomics Proteomics, Bioaster</i> | <b>South Hall 1</b> |
|  | <b>SCIEX</b><br>The portal to multimodal metabolomics and lipidomics<br><i>Prof Nicola Zamboni, Institute of Molecular Systems Biology, ETH Zurich</i>   | <b>South Hall 2</b> |

|                       |   |                      |
|-----------------------|---|----------------------|
| 1:30 p.m. – 3:00 p.m. | <b>Session 7. Data Repositories and Curation</b><br><i>Session Chairs: David Wishart and Fabien Jourdan</i>   | <b>Congress Hall</b> |
| 1:30 p.m. – 1:50 p.m. | <b>7.1</b><br>Three Years of MDCC Efforts in Korea Metabolomics rePository (KMAP): Advancing Metabolomics Data Curation and Global Harmonization<br>★ <i>Woori Chae, Seoul National University, South Korea</i> | <b>121</b>           |
| 1:50 p.m. – 2:05 p.m. | <b>7.2</b><br>MSnLib: High-Throughput Library Generation of 60,000 Compounds in 33 Days<br>★ <i>Corinna Brungs, University of Vienna, Austria</i>   | <b>311</b>           |
| 2:05 p.m. – 2:25 p.m. | <b>7.3</b><br>Lessons from Mass Spectral Library Integration: Addressing Metadata Gaps and Expanding Chemodiversity<br><i>Guillaume Marti, Metabohub, France</i>  | <b>330</b>           |
| 2:25 p.m. – 2:40 p.m. | <b>7.4</b><br>Expanding Reference Data-Driven Metabolomics: A Framework for Enhanced Untargeted Metabolomics Annotation and Interpretability<br><i>Alejandro Mendoza Cantu, University Of Antwerp, Belgium</i>  | <b>177</b>           |
| 2:40 p.m. – 3:00 p.m. | <b>7.5</b><br>IntegMET: An integrated database for knowledge discovery through differential expression re-analysis of existing databases.<br><i>Kozo Nishida, Riken, Japan</i>                                  | <b>359</b>           |

## TECHNOLOGY ADVANCEMENTS

## PLANTS, FOOD, ENVIRONMENT AND MICROBES

### ★ AWARD WINNERS

| Tuesday, June 24             |   |                     |
|------------------------------|---|---------------------|
| Time                         | Session   | Abstract #          |
| <b>1:30 p.m. – 3:00 p.m.</b> | <b>Session 8. Mass Spectrometry Imaging</b><br><i>Session Chairs: Oscar Yanes and Livia Eberlin</i>   | <b>South Hall 1</b> |
| 1:30 p.m. – 1:50 p.m.        | <b>8.1</b><br>Dysregulated sphingolipid metabolism in liver fibrosis: insights from mass spectrometry imaging<br><i>Zoe Hall, Imperial College London, United Kingdom</i>   | <b>167</b>          |
| 1:50 p.m. – 2:05 p.m.        | <b>8.2</b><br>Visualizing the Spatial Landscape of the Brain Endocannabinoidome by MALDI-2-MS Imaging<br><i>Emanuela Salviati, University of Salerno, Italy</i>   | <b>162</b>          |
| 2:05 p.m. – 2:25 p.m.        | <b>8.3</b><br>The effect of the solvent and tissue type on Desorption Electrospray Ionization Mass Spectrometry Imaging of metabolites<br><i>Marco Giampà, Vib/ku Leuven, Belgium</i>   | <b>220</b>          |
| 2:25 p.m. – 2:40 p.m.        | <b>8.4</b><br>Optimized On-Tissue Chemical Derivatization (OTCD) strategy to enhance detection of carboxylic acids and carbonyls on tissue using MALDI-MSI<br>★ <i>Antonia Fecke, Leibniz Institut Für Analytische Wissenschaften, Germany</i>                                | <b>277</b>          |
| 2:40 p.m. – 3:00 p.m.        | <b>8.5</b><br>Spatial Lipidomics with Cyclic Ion Mobility Mass Spectrometry for Resolving Isotopic, Isomeric, and Isobaric molecules in Hepatocellular Carcinoma Tissue<br>★ <i>Pattipong Wisanpitayakorn, Mahidol University, Thailand</i>                                   | <b>292</b>          |
| <b>1:30 p.m. – 3:00 p.m.</b> | <b>Session 9. Microbial Metabolomics</b><br><i>Session Chairs: Sastia Prama Putri and Zdenek Kamenik</i>  | <b>South Hall 2</b> |
| 1:30 p.m. – 1:50 p.m.        | <b>9.1</b><br>Bacterial lipidome discovery through combined metabolic incorporation and mass spectrometric approach<br><i>Xue Li Guan, NTU, Singapore</i>   | <b>190</b>          |
| 1:50 p.m. – 2:05 p.m.        | <b>9.2</b><br>Integrated metabolomics and metagenomics approaches to understanding fluctuations in gut microbial communities and metabolic activity in jersey cows<br>★ <i>Susana Moñino Ramos, SRUC-University of Edinburgh, United Kingdom</i>                              | <b>176</b>          |
| 2:05 p.m. – 2:25 p.m.        | <b>9.3</b><br>Metabolic Interplay Between the Honeybee Gut Microbiota and an Agrochemical Library<br><i>Andrew Quinn, University of Lausanne, Switzerland</i>   | <b>279</b>          |
| 2:25 p.m. – 2:40 p.m.        | <b>9.4</b><br>Comparative metabolomics reveals distinct metabolic adaptations in Crabtree-positive and Crabtree-negative yeast species<br><i>Harini Sridharan, Georgia Institute Of Technology, United States</i>   | <b>508</b>          |
| 2:40 p.m. – 3:00 p.m.        | <b>9.5</b><br>CROSS-FEEDING INTERACTION WITHIN MICROCYSTIS PHYCOSPHERE : New perspectives from the combination of metagenomics, metametabolomics and genome-scale metabolic modeling approaches<br><i>Binta Diémé, Université Clermont Auvergne, INRAE, UNH, PFEM, France</i> | <b>255</b>          |



Tuesday, June 24

| Time                  | Session   | Abstract # |
|-----------------------|---|------------|
| 3:00 p.m. – 3:30 p.m. | <b>BREAK</b>  |            |
| 3:00 p.m. – 3:25 p.m. | <b>BioHub 2</b><br>Metabonaut: A Collection of Tutorials for Learning Metabolomics Data Analysis in R |            |

|                       |   |                      |
|-----------------------|---|----------------------|
| 3:30 p.m. – 5:15 p.m. | <b>Session 10. Vendor Session</b><br>(Presented by Platinum and Gold sponsors)<br><i>Session Chairs: Natasa Giallourou and Aurelia Williams</i> | <b>Congress Hall</b> |
|-----------------------|---|----------------------|

PLATINUM PRESENTERS: 3:30 p.m. – 4:20 p.m.



**SCIEX**

Dr Paul Baker, Senior Staff Scientific Liaison, Lipidomics and Metabolomics, United States  
**Quantitative and qualitative analysis of bile acids by high-resolution mass spectrometry using electron-based fragmentation**



**Thermo Fisher Scientific**

Susan Bird, Vertical Marketing Senior Manager, United States  
**Orbitrap-based Metabolomics workflows: Discover. Innovate. Exceed.**



**Bruker**

Matt Lewis, Ph.D., VP Metabolomics, United Kingdom  
**Discover MORE with Bruker's innovative metabolomics technology portfolio**



**Waters Corporation**

David Heywood, Sr. Manager Omics Market Development, United Kingdom  
**Advancement of flexible high-resolution workflows for Metabolomics and Lipidomics research**



**Agilent**

TBD

Tuesday, June 24

| Time                  | Session   | Abstract #    |
|-----------------------|---|---------------|
| 3:30 p.m. – 5:15 p.m. | <b>Session 10. Vendor Session</b><br>(Presented by Platinum and Gold sponsors)<br><i>Session Chairs: Natasa Giallourou and Aurelia Williams</i> | Congress Hall |

GOLD PRESENTERS: 4:20 p.m. – 5:15 p.m.



Cambridge Isotope  
Laboratories, Inc.  
[isotope.com](http://isotope.com)

**Cambridge Isotope Laboratories**

Dr. Andrew Percy, MS 'Omics Product Manager, United States

**Stable Isotope-Labeled Tools for QC and/or Quantitation in MS Omics**



BECKMAN  
COULTER Life Sciences

**Beckman Coulter Life Sciences**

Rene Goedde, Market Development Manager, Germany

**Enhance Your Metabolomics Research With Automated Liquid Handling**



EMPOWERING RESULTS

**LECO**

Christine Loeb-Stubbins, Field Product Manager Sep Sci Europe, United Kingdom

**Smarter GC-TOF: Sustainable Strategies for High-Throughput Metabolomics**



SHIMADZU  
Excellence in Science

**Shimadzu Europa GmbH**

Emily Armitage, Research Scientist, United Kingdom

**Flexible workflows to enhance metabolomics and lipidomics research**



biocrates  
The future of research and health

**biocrates life sciences ag**

Alice Limonciel, Chief Scientific Officer, Austria

**MxP® Quant 1000 kit - Transform medicine with metabolomics**



cmc Instruments GmbH

**cmc Instruments GmbH**

Rodrigo Aparicio, Head of Brand & Marketing, Germany

**Focusing On Your Analysis: Thinking in gas supply systems for a smooth lab operation in MS & GC**



cmbio

**Cmbio**

Thorsten Gravert, Senior Metabolomics Scientist, Denmark

**Solving Complex Biological Questions with Software-Driven Multi-Omics Integration**



Metabolon  
SMALL MOLECULES, BIG INSIGHTS

**Metabolon**


Brenan Durainayagam, Product Manager, United Kingdom

**Quantify the Exposome: Advancing Precision Health with Metabolomics**

★ **AWARD WINNERS**

| Tuesday, June 24             |  |                     |
|------------------------------|--|---------------------|
| Time                         | Session  | Abstract #          |
| <b>3:30 p.m. – 5:10 p.m.</b> | <b>Session 11. Pregnancy, Neonatal, and Early Life Metabolism</b><br><i>Session Chairs: Julia Kuligowski and David Friedecky</i>   | <b>South Hall 1</b> |
| 3:30 p.m. – 3:50 p.m.        | <b>11.1</b><br>Longitudinal targeted plasma and urine metabolomics reveals novel inositol isomers patterns from preconception into pregnancy<br><i>Jean-Philippe Godin, Nestle Research, Switzerland</i>                             | <b>381</b>          |
| 3:50 p.m. – 4:10 p.m.        | <b>11.2</b><br>Prenatal organophosphate pesticide exposure and the maternal pregnancy metabolome in the NYU CHES cohort<br><i>Haleigh Cavalier, New York University School of Medicine, United States</i>                            | <b>470</b>          |
| 4:10 p.m. – 4:30 p.m.        | <b>11.3</b><br>Metabolomic alterations in cord blood improve the prediction of childhood-onset neurodevelopmental disorders<br><i>Polina Girchenko, University Of Oulu, Finland</i>  | <b>339</b>          |
| 4:30 p.m. – 4:50 p.m.        | <b>11.4</b><br>Early life gut microbial and metabolic shifts reflected in stool consistency<br><i>Santosh Lamichhane, University of Turku, Finland</i>   | <b>312</b>          |
| 4:50 p.m. – 5:10 p.m.        | <b>11.5</b><br>Exploring circulating lipoprotein and metabolite profiles associated with gestational diabetes and offspring outcomes in post-bariatric surgery pregnancies<br><i>Jia Li, Imperial College London, United Kingdom</i> | <b>234</b>          |
| <b>3:30 p.m. – 5:10 p.m.</b> | <b>Session 12. Agricultural and Animal Products</b><br><i>Session Chairs: Kyo Bin Kang and Mónica Cala Molina</i>  | <b>South Hall 2</b> |
| 3:30 p.m. – 3:50 p.m.        | <b>12.1</b><br>Metabolic Profiling of Bovine Colostrum: Unravelling the Influences of Diet and Seasonality on Functional Dairy Components<br><i>Raghunath Pariyani, University College Cork, Ireland, Ireland</i>                    | <b>133</b>          |
| 3:50 p.m. – 4:10 p.m.        | <b>12.2</b><br>Insights from Dual-Platform Metabolomics on Durian Flowers: An Alternative Source of Procyanidins from Agricultural Waste with Bioactivities<br>★ <i>Supakorn Potijun, Chulalongkorn University, Thailand</i>         | <b>338</b>          |
| 4:10 p.m. – 4:30 p.m.        | <b>12.3</b><br>Metabolomic and Microbiota Alterations in Goat Milk During Experimental Subclinical Mastitis by <i>Staphylococcus warneri</i><br>★ <i>Ana Júlia Silva Moreira, Federal University of Viçosa, Brazil</i>               | <b>149</b>          |
| 4:30 p.m. – 4:50 p.m.        | <b>12.4</b><br>Natural variation in the wheat root exudate metabolome and its plant-microbe interactions<br><i>Cristina Lopez-Hidalgo, University of Vienna, Austria</i>   | <b>202</b>          |
| 4:50 p.m. – 5:10 p.m.        | <b>12.5</b><br>Predictive metabolomics to unravel phenotypic traits in pearl millet grains from Brazilian germplasm panel<br>★ <i>Mariana Pinheiro Costa Pimentel, Food and Nutrition Graduate Program (PPGAN-UNIRIO), France</i>    | <b>491</b>          |


## ★ AWARD WINNERS

| Wednesday, June 25      |  |                      |
|-------------------------|--|----------------------|
| Time                    | Session  | Abstract #           |
| 8:30 a.m. – 9:30 a.m.   | <b>Plenary Session 3</b><br><i>Steffen Neumann, Leibniz Institute of Plant Biochemistry, Germany</i><br>Hitchhiker's Guide to Computational Metabolomics   | <b>Congress Hall</b> |
| 9:30 a.m. – 10:15 a.m.  | <b>BREAK</b>   |                      |
| 9:40 a.m. – 10:10 a.m.  | <b>BioHub 3</b><br>Empowering GC-MS metabolomics with PARADISe   |                      |
| 9:45 a.m. – 10:00 a.m.  | <b>EXHIBITOR DEMO PRESENTATION – GOLD SPONSOR</b><br><b>Metabolon</b><br>Microbiome Research Solution Demo<br><i>Brenan Durainayagam, Ph.D., Product Manager</i>   |                      |
|                         |   |                      |
| 10:15 a.m. – 12:00 p.m. | <b>Session 13. Multi-omics and Integrative Methods</b><br><i>Session Chairs: Justin JJ van der Hooft and Wout Bittremieux</i>  | <b>Congress Hall</b> |
| 10:15 a.m. – 10:45 a.m. | <b>13.1 KEYNOTE</b><br>Multi-modal exploration for plasma biomarkers of post-MI major adverse cardiovascular outcomes in New Zealand and Singapore – computational tools, lessons and the vision forward.<br><i>Hyungwon Choi, National University Of Singapore, Singapore</i> | <b>353</b>           |
| 10:45 a.m. – 11:05 a.m. | <b>13.2</b><br>Integration of Omics and Spectroscopic Data for Enhanced Prediction of HCC<br><i>Antonio Malinconico, University of Naples Federico II, Italy</i>   | <b>461</b>           |
| 11:05 a.m. – 11:25 a.m. | <b>13.3</b><br>Multi-omics integration reveals restored and resistant liver metabolic pathways following a lifestyle intervention in mice<br>★ <i>Jordi Rofes, Universitat Rovira i Virgili, Spain</i>   | <b>252</b>           |
| 11:25 a.m. – 11:45 a.m. | <b>13.4</b><br>Using optimal transport to integrate spatial multiomics data<br><i>Nami Sakamoto, Tokyo University of Agriculture and Technology, Japan</i>   | <b>241</b>           |
| 11:45 a.m. – 12:00 p.m. | <b>13.5</b><br>Metabolomic and Integrative Analysis of COVID-19 and Long-COVID Based on ISARIC and PHOSP-COVID Studies<br><i>Desai Chen, Imperial College London, United Kingdom</i>   | <b>499</b>           |

★ **AWARD WINNERS**

| Wednesday, June 25             |   |                     |
|--------------------------------|---|---------------------|
| Time                           | Session   | Abstract #          |
| <b>10:15 a.m. – 12:00 p.m.</b> | <b>Session 14. Microbiome and Host-Metabolism Interactions</b><br><i>Session Chairs: Anna Halama and Caroline Johnson</i>   | <b>South Hall 1</b> |
| 10:15 a.m. – 10:45 a.m.        | <b>14.1 KEYNOTE</b><br>Poo, piss and plasma: the dirtier side of exploring the role of metabolites in inflammatory disease<br><i>Jennifer Kirwan, Berlin Inst. Of Health At Charite, Germany</i>  | <b>571</b>          |
| 10:45 a.m. – 11:05 a.m.        | <b>14.2</b><br>Mapping microbial lipid production: the impact of linoleic acid on gut microbiota composition and function<br><i>Josep Rubert, Wageningen University And Research, Netherlands</i>   | <b>161</b>          |
| 11:05 a.m. – 11:25 a.m.        | <b>14.3</b><br>Metabolomics-guided discovery of novel antibiotics from the human microbiome<br><i>Karin Meier, Roche, Switzerland</i>   | <b>111</b>          |
| 11:25 a.m. – 11:45 a.m.        | <b>14.4</b><br>A prebiotic diet intervention can restore faecal short chain fatty acids in Parkinson's Disease yet fails to restore the gut metabolome and microbiome homeostasis<br><i>Silke Heinzmann, Helmholtz Munich, Germany</i>    | <b>445</b>          |
| 11:45 a.m. – 12:00 p.m.        | <b>14.5</b><br>Herpesvirus exposures are associated with disrupted phospholipid metabolite profiles and incidence of chronic inflammatory diseases<br>★ <i>Nicole Prince, Brigham &amp; Women's Hospital, United States</i>               | <b>199</b>          |
| <b>10:15 a.m. – 12:00 p.m.</b> | <b>Session 15. Natural Products and Plant Defense</b><br><i>Session Chairs: Jing-Ke Weng and Ondrej Novak</i>   | <b>South Hall 2</b> |
| 10:15 a.m. – 10:45 a.m.        | <b>15.1 KEYNOTE</b><br>Advances in Chemical Ecology and Mass Spectrometry: Unraveling Natural Products in Biological Communication<br><i>Norberto Pepporine Lopes, University Of São Paulo, Brazil</i>                                    | <b>303</b>          |
| 10:45 a.m. – 11:05 a.m.        | <b>15.2</b><br>Plant Defense in Monocots: A Multi-Bladed Swiss Knife with Conserved Metabolic Traits?<br><i>Gerd U. Balcke, IPB-Halle, Germany</i>  | <b>375</b>          |
| 11:05 a.m. – 11:25 a.m.        | <b>15.3</b><br>Exploring the Mode of Action of 20 Mycotoxins using a Powerful Targeted Metabolomics Approach<br>★ <i>Andrea Gerdemann, University of Muenster, Germany</i>  | <b>501</b>          |
| 11:25 a.m. – 11:45 a.m.        | <b>15.4</b><br>A combination of Untargeted Metabolomics and Mass Spectral Imaging: A case study on the interaction between Eucalyptus species and the weevil Gonipterus platensis.<br><i>Andy Pérez, Universidad De Concepcion, Chile</i> | <b>138</b>          |
| 11:45 a.m. – 12:00 p.m.        | <b>15.5</b><br>Exploring Grapevine Metabolomics: Pathogen Interactions and Defense Pathways<br><i>Marisa Maia, FCIências.ID - Associação para a Investigação e Desenvolvimento de Ciências, Portugal</i>                                  | <b>331</b>          |

## ★ AWARD WINNERS


| Wednesday, June 25   |   |                      |
|--|---|----------------------|
| Time   | Session   | Abstract #           |
| 12:20 p.m. – 1:20 p.m.   | <b>Sponsor Lunch Presentations</b>  |                      |
|   | <p><b>Waters Corporation</b><br/> Lipid Metabolism in Traumatic Brain Injury – Increased identification confidence whilst extending coverage with the Waters Xevo™ MRT<br/> <i>Dr. Elizabeth Want, Reader in Clinical Mass Spectrometry, Imperial College London</i></p> <p>Parallel targeted and untargeted metabolite analysis of mouse plasma samples using a benchtop multi-reflecting time of flight mass spectrometer<br/> <i>Dr. Adam King, Senior Scientist, Waters Corporation</i></p> | <b>South Hall 1</b>  |
|  | <p><b>Bruker</b><br/> TIMS-enabled Lipidomics: Explore high-sensitivity lipidomics<br/> <i>Dr. Michael Witting, Metabolomics and Proteomics Core, Helmholtz Munich</i></p> <p>LC- and NMR-supported Metabolomics: Discover groundbreaking data and insights<br/> <i>Dr. Christoph Trautwein, Director Core Facility Metabolomics, University of Tuebingen</i></p>   | <b>South Hall 2</b>  |
| 1:30 p.m. – 3:00 p.m.  | <b>Session 16. Age-Related Diseases and Cancer</b><br><i>Session Chairs: Matej Oresic and Elizabeth Want</i>  | <b>Congress Hall</b> |
| 1:30 p.m. – 1:50 p.m.  | <b>16.1</b><br>Decoding Alzheimer's Disease Through Brain Metabolomics: Metabolic Dysregulation and Pathway Insights<br><i>Donghai Liang, Emory University, United States</i>   | <b>324</b>           |
| 1:50 p.m. – 2:05 p.m.  | <b>16.2</b><br>Metabolomics and Aging: Identifying Biomarkers of Obesity, Diabetes, and Hypertension<br><i>Anas Abdel Rahman, King Faisal Specialist Hospital &amp; Research Centre, Saudi Arabia</i>   | <b>213</b>           |
| 2:05 p.m. – 2:25 p.m.  | <b>16.3</b><br>Dissecting Metabolic Alterations in Pancreatic Cancer<br>★ <i>Carolin Schneider, M3 Research Center, Germany</i>   | <b>452</b>           |
| 2:25 p.m. – 2:40 p.m.  | <b>16.4</b><br>Baseline Serum Metabolomic Profiling Identifies 3-Hydroxybutyrate and Acetone as Prognostic Biomarkers in Relapsed/Refractory DLBCL Patients Treated with R2-GDP<br><i>Joan Badia Cabré, Institut d'Investigació Sanitària Pere Virgili (IISPV), Spain</i>   | <b>466</b>           |
| 2:40 p.m. – 3:00 p.m.  | <b>16.5</b><br>Metabolomic Profiles for Ovarian Cancer Early Detection<br><i>Oana Alina Zeleznik, Harvard Medical School and Brigham &amp; Women's Hospital, United States</i>  | <b>95</b>            |



★ AWARD WINNERS

| Wednesday, June 25           |  |                     |
|------------------------------|--|---------------------|
| Time                         | Session  | Abstract #          |
| <b>1:30 p.m. – 3:00 p.m.</b> | <b>Session 17. Biomonitoring and Environmental Metabolomics</b><br><i>Session Chairs: Gunda Koellensperger and Millena Barros-Santos</i>   | <b>South Hall 1</b> |
| 1:30 p.m. – 1:50 p.m.        | <b>17.1</b><br>Don't Smile at a Polluted Crocodile: PFAS Contamination and its Impact on wild-caught Australian Saltwater Crocodiles ( <i>Crocodylus porosus</i> )<br><i>David Beale, CSIRO, Australia</i>                                 | <b>219</b>          |
| 1:50 p.m. – 2:05 p.m.        | <b>17.2</b><br>Using 18O-assisted phosphometabolomics to elucidate key enzymatic pathways regulating cellular phosphorus metabolism under stress<br>★ <i>Cheng Shi, Eawag, Switzerland</i>   | <b>259</b>          |
| 2:05 p.m. – 2:25 p.m.        | <b>17.3</b><br>1H NMR metabolomics and embryotoxicity tests: Insights into the effects of polystyrene microplastics and bisphenol A in the black sea urchin <i>Arbacia lixula</i><br><i>Tiziana Cappello, University of Messina, Italy</i> | <b>503</b>          |
| 2:25 p.m. – 2:40 p.m.        | <b>17.4</b><br>Global meta-metabolomics reveals marine chemical diversity<br>★ <i>Maia Henry, Friedrich Schiller Universität, Germany</i>  | <b>217</b>          |
| 2:40 p.m. – 3:00 p.m.        | <b>17.5</b><br>Metabolomics for monitoring seagrass responses along a nutrient gradient<br><i>Steven Melvin, Griffith University, Australia</i>  | <b>117</b>          |
| <b>1:30 p.m. – 3:00 p.m.</b> | <b>Session 18. Metabolomics Beyond LC-MS: NMR and More</b><br><i>Session Chairs: Roy Goodacre and Warwick Dunn</i>   | <b>South Hall 2</b> |
| 1:30 p.m. – 1:50 p.m.        | <b>18.1</b><br>NMR-Based Metabolomics to Investigate the Coupling of Arginine Methylation and Metabolism<br><i>Tobias Madl, Medical University of Graz, Austria</i>  | <b>171</b>          |
| 1:50 p.m. – 2:05 p.m.        | <b>18.2</b><br>Metabolomic Insights into Amphetamine-Type Stimulant Misuse: Unraveling Biochemical Pathways and Biomarkers<br><i>Ruzmayuddin Mamat, University Malaya Centre For Addiction Science, Malaysia</i>                           | <b>29</b>           |
| 2:05 p.m. – 2:25 p.m.        | <b>18.3</b><br>Measurement of isotopologue ratios for metabolic flux analysis via parallel, quasi-simultaneous EI and CI-TOFMS detection with a novel, flexible CI source<br><i>Pegah Mousazadehfazeli, BOKU University, Austria</i>       | <b>446</b>          |
| 2:25 p.m. – 2:40 p.m.        | <b>18.4</b><br>In vivo real-time metabolic isotopic tracing via breath analysis upon deuterated water ingestion<br><i>Zhihong Yin, University of Basel, Switzerland</i>  | <b>361</b>          |
| 2:40 p.m. – 3:00 p.m.        | <b>18.5</b><br>Multum in parvo: how to derive three one-dimensional NMR spectra from a single acquired spectrum<br><i>Leonardo Tenori, University Of Florence, Italy</i>   | <b>342</b>          |

## ★ AWARD WINNERS

| Wednesday, June 25    |  |                      |
|-----------------------|--|----------------------|
| Time                  | Session  | Abstract #           |
| 3:00 p.m. – 3:30 p.m. | <b>BREAK</b>   |                      |
| 3:00 p.m. – 3:25 p.m. | <b>BioHub 4</b><br>Metabolomics data processing, analysis and metabolite identification using Metabox 2.0 and SiMD   |                      |
| 3:10 p.m. – 3:25 p.m. | <b>EXHIBITOR DEMO PRESENTATION – PLATINUM SPONSOR</b><br><b>Thermo Fisher Scientific</b><br>Compound Discoverer 3.4: Smarter. Better. Faster. Stronger.<br><i>Ralf Tautenhahn, Product Manager, Metabolomics Software</i>    |                      |
|                       |   |                      |
| 3:30 p.m. – 5:10 p.m. | <b>Session 19. Metabolite Annotation</b><br><i>Session Chairs: Steffen Neumann and Laura Goracci</i>   | <b>Congress Hall</b> |
| 3:30 p.m. – 3:50 p.m. | <b>19.1</b><br>Reverse metabolomics enables public data mining and identifies a drug–bile acid conjugate in inflammatory diseases<br><i>Vincent Charron-lamoureux, University Of California San Diego, United States</i>     | <b>406</b>           |
| 3:50 p.m. – 4:10 p.m. | <b>19.2</b><br>Twin neural network-based spectrum transformer for small molecule analog discovery from untargeted mass spectrometry<br>★ <i>Juan Sebastian Piedrahita Giraldo, University of Antwerp, Belgium</i>            | <b>86</b>            |
| 4:10 p.m. – 4:30 p.m. | <b>19.3</b><br>Interpreting 200 million metabolite mass spectra using DreaMS-Net – a neural network-based molecular networking<br><i>Roman Bushuiev, IOCB Prague, Czechia</i>  | <b>196</b>           |
| 4:30 p.m. – 4:50 p.m. | <b>19.4</b><br>Novel transformation product annotation with SIRIUS – Combining spectral libraries and structure databases<br><i>Markus Fleischauer, Friedrich Schiller University Jena, Germany</i>                          | <b>471</b>           |
| 4:50 p.m. – 5:10 p.m. | <b>19.5</b><br>MVP-JESTR: MultiView Projection-Joint Embedding Space Technique for Ranking Candidate Molecules for the Annotation of Untargeted Metabolomics Data<br>★ <i>Yan Zhou Chen, Tufts University, United States</i> | <b>187</b>           |

★ **AWARD WINNERS**

| Wednesday, June 25           |   |                     |
|------------------------------|---|---------------------|
| Time                         | Session   | Abstract #          |
| <b>3:30 p.m. – 5:10 p.m.</b> | <b>Session 20. Cardiovascular &amp; Endocrine Disease</b><br><i>Session Chairs: Anne Bendt and Aleš Kvasnička</i>   | <b>South Hall 1</b> |
| 3:30 p.m. – 3:50 p.m.        | <b>20.1</b><br>Metabolome-wide association of carotid intima media thickness identifies ferredoxin (FDX1) as a determinant of cholesterol metabolism and cardiovascular risk in Asian populations.<br>★ <i>Nilanjana Sadhu, Nanyang Technological University, Singapore</i> | <b>77</b>           |
| 3:50 p.m. – 4:10 p.m.        | <b>20.2</b><br>Lipidomic profiles and their relationship to incident diabetic retinopathy in type 2 diabetes: The Fremantle Diabetes Study Phase II<br><i>Nicola Gray, Murdoch University, Australia</i>  | <b>432</b>          |
| 4:10 p.m. – 4:30 p.m.        | <b>20.3</b><br>Untargeted tracer-based multi-omics identifies a novel role for pyruvate dehydrogenase kinase 1 (PDK1) in cardiomyocyte metabolism.<br><i>Michael Atser, University Of British Columbia, Canada</i>  | <b>238</b>          |
| 4:30 p.m. – 4:50 p.m.        | <b>20.4</b><br>NAD <sup>+</sup> Depletion Drives Metabolic Dysfunction in Diabetic Kidney Disease: Integrating Clinical Biomarkers with Mechanistic Insights<br><i>Jianhong Ching, Duke-NUS Medical School, Singapore</i>   | <b>302</b>          |
| 4:50 p.m. – 5:10 p.m.        | <b>20.5</b><br>Lipid metabolism drives diet-influenced metabolic health: insights from high-throughput profiling of 10,339 individuals in the Australian Obesity, Diabetes, and Lifestyle Study<br>★ <i>Habtamu Beyene, Baker Heart And Diabetes Institute, Australia</i>   | <b>59</b>           |
| <b>3:30 p.m. – 5:10 p.m.</b> | <b>Session 21. Going Small – Low Volume and Low Sample Amount</b><br><i>Session Chairs: Michael Witting and Boryana Petrova</i>   | <b>South Hall 2</b> |
| 3:30 p.m. – 3:50 p.m.        | <b>21.1</b><br>A multi-omics method for the study of plant natural product biosynthesis in single cells<br><i>Lorenzo Caputi, Max-Planck Institute For Chemical Ecology, Germany</i>  | <b>334</b>          |
| 3:50 p.m. – 4:10 p.m.        | <b>21.2</b><br>Subcellular lipidome and proteome profiling utilizing one-pot lipidomic/proteomic organelle immuno-precipitation<br><i>Brian DeFelice, CZ Biohub – San Francisco, United States</i>  | <b>289</b>          |
| 4:10 p.m. – 4:30 p.m.        | <b>21.3</b><br>Can blood microsampling devices rival plasma for metabolomics?<br><i>Daniel Marques De Sa e Silva, Greece</i>  | <b>197</b>          |
| 4:30 p.m. – 4:50 p.m.        | <b>21.4</b><br>Microflow liquid chromatography coupled to multinozzle electrospray ionization mass spectrometry for discovery lipidomics<br><i>Isabel Meister, University of Geneva, Switzerland</i>  | <b>362</b>          |
| 4:50 p.m. – 5:10 p.m.        | <b>21.5</b><br>Rapid Microbore Metabolic Profiling (RAMMP) for High-Throughput Lipid Analysis in Blood Microsampling Devices<br><i>Ana Sanchez Lorenzo, Imperial College London, United Kingdom</i>   | <b>350</b>          |


## ★ AWARD WINNERS

| Thursday, June 26       |   |                      |
|-------------------------|---|----------------------|
| Time                    | Session   | Abstract #           |
| 8:30 a.m. – 9:30 a.m.   | <b>Plenary Session 4</b><br><i>Peter Meikle, Baker Heart And Diabetes Institute, Australia</i><br>Plasma lipidomic profiling of large population cohorts: Development of a precision medicine approach to cardiometabolic disease                                       | <b>Congress Hall</b> |
| 9:30 a.m. – 10:30 a.m.  | <b>BREAK</b>  |                      |
| 9:40 a.m. – 10:10 a.m.  | <b>BioHub 5</b><br>MSlineaR: a new R package to assess linearity, improving statistical robustness and quality assurance in untargeted metabolomics   |                      |
| 10:30 a.m. – 12:15 p.m. | <b>Session 22. Nutrition and Exposome Research</b><br><i>Session Chairs: Sandi Azab and Kati Hanhineva</i>  | <b>Congress Hall</b> |
| 10:30 a.m. – 11:00 a.m. | <b>22.1 KEYNOTE</b><br>Unveiling Diet–Health Links: The Power of Diverse Study Designs in Precision Nutrition, Recent Advances in the Application of Metabolomics for Nutrition and Health<br><i>Cristina Andres-lacueva, University of Barcelona – Ciberfes, Spain</i> | <b>550</b>           |
| 11:00 a.m. – 11:20 a.m. | <b>22.2</b><br>Finger sweat analysis enables individual metabolic monitoring of nutritional intervention<br>★ <i>Daniel Wasinger, University Of Vienna, Austria</i>   | <b>378</b>           |
| 11:20 a.m. – 11:40 a.m. | <b>22.3</b><br>Metabolomic and transcriptomic signatures of steatotic liver disease, with focus on sex-specific impacts of PFAS<br><i>Matej Orešič, Örebro University, Sweden</i>   | <b>336</b>           |
| 11:40 a.m. – 12:00 p.m. | <b>22.4</b><br>Early life exposure to endocrine disruptors: Understanding the neuro-endocrine impact from metabolome mapping of rat models<br><i>Pim Leonards, Vrije Universiteit Amsterdam, Netherlands</i>  | <b>183</b>           |
| 12:00 p.m. – 12:15 p.m. | <b>22.5</b><br>Comprehensive characterisation of children’s exposure to air pollutants using personal samplers and a multiplatform High-Resolution Mass Spectrometry approach<br>★ <i>Camilla Guerrini, Universitat Rovira i Virgili, Spain</i>                         | <b>479</b>           |

## ★ AWARD WINNERS

| Thursday, June 26              |  |                     |
|--------------------------------|--|---------------------|
| Time                           | Session  | Abstract #          |
| <b>10:30 a.m. – 12:15 p.m.</b> | <b>Session 23. Food, Health, and Sustainability</b><br><i>Session Chairs: Lynn Vanhaecke and Eiichiro Fukusaki</i>   | <b>South Hall 1</b> |
| 10:30 a.m. – 11:00 a.m.        | <b>23.1 KEYNOTE</b><br>Efficient identification of underexplored health-promoting metabolites through integration of food and human metabolome data and nutritional epidemiology<br><i>Sastia Prama Putri, Osaka University, Japan</i> | <b>551</b>          |
| 11:00 a.m. – 11:20 a.m.        | <b>23.2</b><br>1H NMR spectral database for Czech wine quality control<br><i>Jaroslav Havlik, Ceska Zemedelska Univerzita v Praze, Czech Republic</i>  | <b>462</b>          |
| 11:20 a.m. – 11:40 a.m.        | <b>23.3</b><br>Unlocking the potential of metabolomics for comprehensive insights into edible insects<br><i>Kateřina Šebelová, University of Chemistry and Technology, Czech Republic</i>  | <b>428</b>          |
| 11:40 a.m. – 12:00 p.m.        | <b>23.4</b><br>Decoding the Geographical Origins of Tea: A Machine Learning Driven Untargeted Metabolomics Approach for Fraud Detection<br>★ <i>Yicong Li, Queens University Belfast, United Kingdom</i>                               | <b>143</b>          |
| 12:00 p.m. – 12:15 p.m.        | <b>23.5</b><br>Lipidomic Analysis Unveils <i>S. maritima</i> as a Sustainable Source of Food Lipids through Hydroponic Cultivation<br><i>Marisa Pinho, University Of Aveiro, Portugal</i>  | <b>320</b>          |

## ★ AWARD WINNERS

| Thursday, June 26  |  |                      |
|--|--|----------------------|
| Time   | Session  | Abstract #           |
| 10:30 a.m. – 12:10 p.m.  | <b>Session 24. Data Processing and Cheminformatics</b><br><i>Session Chairs: Tomáš Pluskal and Niek de Jonge</i>   | <b>South Hall 2</b>  |
| 10:30 a.m. – 10:50 a.m.  | <b>24.1</b><br>RforMassSpectrometry: A Community-Driven Ecosystem for Reproducible and Scalable Mass Spectrometry Data Analysis in R – Join Us, We Have Spectra!<br><i>Johannes Rainer, Eurac Research, Italy</i>  | <b>89</b>            |
| 10:50 a.m. – 11:10 a.m.  | <b>24.2</b><br>xcms at 20 and still in Peak form: Now anchoring a complete ecosystem for metabolomics data preprocessing and analysis.<br><i>Philippine Louail, Institute for Biomedicine, Eurac Research, Italy</i>   | <b>163</b>           |
| 11:10 a.m. – 11:30 a.m.  | <b>24.3</b><br>Multiplet Matching in Metabolomic J-Res NMR Spectra using Deep Learning Video Networks<br><i>Yan Yan, Imperial College London, United Kingdom</i>   | <b>275</b>           |
| 11:30 a.m. – 11:50 a.m.  | <b>24.4</b><br>LipidCXSMILES: A dynamic solution to represent lipid structures towards the “Dark Matter” discovery<br><i>Zhixu Ni, TU Dresden, Germany</i>   | <b>396</b>           |
| 11:50 a.m. – 12:10 p.m.  | <b>24.5</b><br>Deep Learning-Assisted Single-Cell Data Processing Platform for Metabolite Profiling<br>★ <i>Felix Friedrich, Uppsala University, Sweden</i>  | <b>131</b>           |
| 12:25 p.m. – 1:25 p.m.   | <b>Sponsor Lunch Presentation</b>  |                      |
|  <b>Agilent</b> | <b>Agilent Technologies</b><br>Combining Cellular Bioenergetics with Metabolomics. Take your metabolomics workflow to the next level.<br><i>Daniel Cuthbertson, Director, Global Life Science Research Market, Agilent Technologies</i><br><i>David Beale, Senior Research Scientist, Adjunct Professor of RMIT University</i> | <b>South Hall 2</b>  |
| 1:30 p.m. – 3:15 p.m.  | <b>Plenary Session 5   Awards &amp; Closing</b><br><i>Clary Clish, Broad Institute Of MIT And Harvard, United States</i><br>Discovery of metabolic indicators of disease, outcomes, and health in human cohorts using nontargeted metabolomics: approaches, challenges, and opportunities.                                     | <b>Congress Hall</b> |