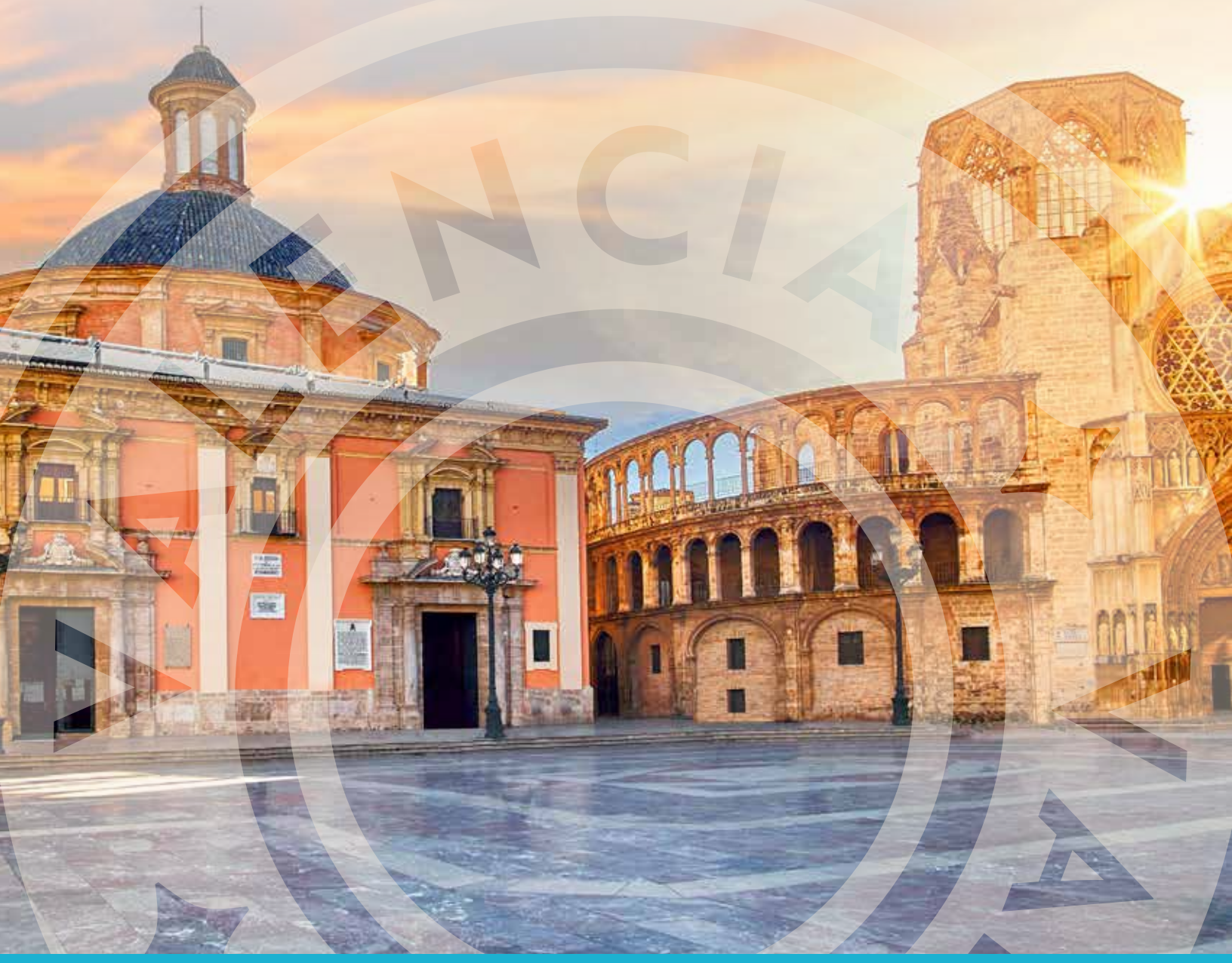
METABOLOMICS SOCIETY

18th Annual Conference of the Metabolomics Society

# METABOLOMICS 2022

## Valencia, Spain | JUNE 19-23



# SCHEDULE OF ORAL PRESENTATIONS

# AGENDA AT A GLANCE

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

## SUNDAY, JUNE 19

| | Auditorium 2 | MP 1 – AB | MP 1 – CD |
|---|---|---|---|
| 11:00 a.m. | REGISTRATION OPEN | | |
| 12:00 p.m. – 2 p.m. | **W1:** Ion Mobility in Metabolomics: New Tech and Workflows | **W2:** Spectra Processing Using MetaboAnalyst 5.0 Part 1 | |
| 2:15 p.m. – 4:15 p.m. | **W3:** Mass Spectrometry Data Processing with MZmine 3 | **W2 Cont:** Spectra Processing Using MetaboAnalyst 5.0 Part 2 | **W4:** Frontiers in NMR Metabolomics |
| 4:30 p.m. – 6:30 p.m. | **W5:** State of QA/QC Best Practices in LC-MS-Based Untargeted Metabolomics | **W6:** EMN Professional Career Development | **W7:** Towards Spatial Metabolomics |
| 6:30 p.m. – 8:30 p.m. | **Career Night** | | |

## MONDAY, JUNE 20

| | Auditorium 2 | MP 1 – AB | MP 1 – CD |
|---|---|---|---|
| 7:45 a.m. | REGISTRATION / INFO DESK OPEN | | |
| 8:15 a.m. – 10:15 a.m. | **W8:** Clinical Lipidomics | **W9:** Mining the Metabolome Using the Mass Spec Query | **W10:** Hitchhikers' Guide to Networks in Metabolomics |
| 10:30 a.m. – 12:30 p.m. | **W11:** The 3 R's of Effective Data Sharing in Metabolomic Epidemiology | **W12:** Revisiting CASMI: compound ID for 500 new unknowns, using LC-MS/MS data | **W13:** Big Data Machine Learning Methods for Metabolomics |
| | LUNCH BREAK – ON YOUR OWN | | |
| 1:30 p.m. – 3 p.m. | **Welcome and Opening Plenary Session –** Ron Heeren | | |
| 3 p.m. – 3:30 p.m. | BREAK | | |
| | **Auditorium 2** | **Auditorium 1** | **MP 1** |
| 3:30 p.m. – 5:15 p.m. | **1** Epidemiology | **2** Computational Metabolomics Workflows | **3** Foodomics |
| 5:15 p.m. – 6:45 p.m. | **Welcome Reception – Poster Session 1** | | |
| 7:00 p.m. – 8:00 p.m. | **Metabolomics Society Town Hall Meeting** | | |

## TUESDAY, JUNE 21

| | Auditorium 1 | Auditorium 2 | MP 1 |
|---|---|---|---|
| 7:45 a.m. | REGISTRATION / INFO DESK OPEN | | |
| 8:30 a.m. – 9:30 a.m. | **Plenary Session 2 –** Nicola Zamboni | | |
| 9:30 a.m. – 10:15 a.m. | BREAK | | |
| 10:15 a.m.– 12 p.m. | **4** Neurological Disorders | **5** Data Analysis and Modeling | **6** Plant Metabolomics |
| 12 p.m. – 1:30 p.m. | LUNCH BREAK AND SPONSOR PRESENTATIONS | | |
| 12:20 p.m. – 1:20 p.m. | **Sponsor Pres:** Bruker | **Sponsor Pres:** SCIEX | |
| 1:30 p.m. – 3 p.m. | **7** Infectious Diseases | **8** MetID I | **9** Technology Advancements I |
| 3 p.m. – 3:30 p.m. | BREAK | | |
| 3:30 p.m. – 5 p.m. | **10** Lipidomics and Cardiovascular Diseases | **11** Vendor Session | **12** Plant and Environmental Applications I |
| 5 p.m. – 6:30 p.m. | **Poster Session 2** | | |
| 6:45 p.m. – 8:15 p.m. | **EMN Reception** | | |

## WEDNESDAY, JUNE 22

| | Auditorium 1 | Auditorium 2 | MP 1 |
|---|---|---|---|
| 8:00 a.m. | REGISTRATION / INFO DESK OPEN | | |
| 8:30 a.m. – 9:30 a.m. | **Plenary Session 3** – Asaph Aharoni | | |
| 9:30 a.m. – 10:15 a.m. | BREAK | | |
| 10:15 a.m. – 12 p.m. | **13** Cancer | **14** Collaborative Data Science & Cloud Computing | **15** Technology Advancements II |
| 12 p.m. – 1:30 p.m. | LUNCH BREAK – ON YOUR OWN | | |
| 12:20 p.m. – 1:20 p.m. | **Sponsor Pres:** Agilent | **Sponsor Pres:** Thermo Fisher Scientific | |
| 1:30 p.m. – 3 p.m. | **16** Lung and Respiratory Diseases | **17** Plant and Environmental Applications II | **18** QA/QC and Reproducibility |
| 3 p.m. – 3:30 p.m. | BREAK | | |
| 3:30 p.m. – 5 p.m. | **19** Metabolomics Throughout the Lifecourse | **20** MetID II | **21** Metabolic Diseases |
| 5:15 p.m. – 6:45 p.m. | **Poster Session 3** | | |
| 7:30 p.m. – 10:30 p.m. | **Conference Dinner** | | |

## THURSDAY, JUNE 23

| | Auditorium 1 | Auditorium 2 | MP 1 |
|---|---|---|---|
| 8:15 a.m. | REGISTRATION / INFO DESK OPEN | | |
| 8:30 a.m. – 10:15 a.m. | **22** Microbiome and Gastrointestinal Function | **23** Natural Products | **24** Analytical Methods in Lipidomics |
| 10:15 a.m. – 11:30 a.m. | **Poster Session 4** | | |
| 11:30 a.m. – 1 p.m. | **Plenary Session 4** – Coral Barbas – **Awards and Closing** | | |
| 1 p.m. | BOX LUNCH TO GO | | |

## METABOLOMICS IN HEALTH AND DISEASE
## COMPUTATIONAL METABOLOMICS, STATISTICS & BIOINFORMATICS

***AWARD WINNERS**

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

***AWARD WINNERS**

| Monday, June 20 | | |
|---|---|---|
| **Time** | **Session** | **Abstract #** |
| **3:30 p.m. – 5:15 p.m.** | **Session 3. Foodomics**<br>*Session Chairs: Kati Hanhineva and Kang Chen* | *Multi Purpose 1* |
| 3:30 p.m. – 4 p.m. | **3.1 KEYNOTE**<br>Untargeted Metabolomics as a valuable Tool for quality Improvement of Fine-flavor cocoa and Coffee beverages during food processing<br>*Monica Cala, Universidad de Los Andes, Colombia* | **471** |
| 4 p.m. – 4:20 p.m. | **3.2**<br>Metabolomics reveals the chemical dynamics in green and white asparagus<br>*Robert Hall, Wageningen University & Research, Netherlands* | **282** |
| 4:20 p.m. – 4:35 p.m. | **3.3**<br>Application of FTIR spectroscopy in tandem with machine learning for the microbiological quality assessment and discrimination of various types of mussels<br>*Anastasia Lytou, Agricultural University Of Athens, Greece* | **335** |
| 4:35 p.m. – 4:55 p.m. | **3.4**<br>Lipidomic profiling of bioactive lipids during spontaneous fermentation of fine-flavour cocoa<br>**Miguel Fernández-Niño, Leibniz Institute of Plant Biochemistry: Halle Neustadt, DE, Colombia* | **215** |
| 4:55 p.m. – 5:10 p.m. | **3.5**<br>A foodomics study on the molecular composition of cooking vapor from the processing of foodstuff<br>*Leopold Weidner, Technical University Of Munich, Germany* | **64** |

***AWARD WINNERS**

| Tuesday, June 21 | | |
|---|---|---|
| **Time** | **Session** | **Abstract #** |
| **8:30 a.m. – 9:30 a.m.** | **Plenary Session 2**<br>Democratization of untargeted metabolomics for integration in discovery and clinical workflows<br>*Nicola Zamboni, ETH Zurich, Switzerland* | *Auditorium 1* |
| **10:15 a.m. – 12 noon** | **Session 4. Neurological Disorders**<br>*Session Chairs: Tuulia Hyötyläinen and Sofina Begum* | *Auditorium 1* |
| 10:15 a.m. – 10:45 a.m. | **4.1 SESSION KEYNOTE**<br>Immune activation, neurodevelopment, and risk of offspring ADHD: a survey of the circulating maternal metabolome during pregnancy<br>*Su Chu, Brigham and Women's Hospital and Harvard Medical School, United States* | **340** |
| 10:45 a.m. – 11:05 a.m. | **4.2**<br>The circulating metabolome associates with severity of acute traumatic brain injury, computed tomography findings, and patient outcomes<br>*Matej Oresic, Örebro University, Sweden* | **267** |
| 11:05 a.m. – 11:20 a.m. | **4.3**<br>Novel CSF biomarkers of GLUT1 deficiency syndrome: implications beyond the brain's energy deficit<br>**Tessa Peters, Radboudumc, Netherlands* | **87** |
| 11:20 a.m. – 11:40 a.m. | **4.4**<br>Identification of neurodegeneration indicators and disease progression in metachromatic leukodystrophy using quantitative NMR-based urinary metabolomics<br>*Christoph Trautwein, University Of Tuebingen, Germany* | **330** |
| 11:40 a.m. – 11:55 a.m. | **4.5**<br>Targeted Metabolomic and Lipidomic Analysis in Parkinson's Disease Brain Tissue Across Spectrum of Cognitive Impairment<br>*Karel Kalecký, Baylor University, United States* | **360** |
| **10:15 a.m. – 12 noon** | **Session 5. Data Analysis and Modeling**<br>*Session Chairs: Serge Rudaz and Yann Guitton* | *Auditorium 2* |
| 10:15 a.m. – 10:45 a.m. | **5.1 KEYNOTE**<br>Democratizing metabolomics through new-generation computing framework<br>*Jianguo (Jeff) Xia, McGill University, Canada* | **422** |
| 10:45 a.m. – 11:05 a.m. | **5.2**<br>FAMetA: a mass-isototopogue-based tool for the comprehensive analysis of fatty acid metabolism<br>*Juan Carlos Garcia Cañaveras, IIS-La Fe, Spain* | **265** |
| 11:05 a.m. – 11:20 a.m. | **5.3**<br>Performance evaluation and applicability of single-sample pathway analysis methods to metabolomics data<br>*Cecilia Wieder, Imperial College London, United Kingdom* | **102** |
| 11:20 a.m. – 11:40 a.m. | **5.4**<br>XomicsToModel: Multiomic data integration and generation of thermodynamically consistent metabolic models<br>*Ronan Fleming, Leiden University, Netherlands* | **42** |
| 11:40 a.m. – 11:55 a.m. | **5.5**<br>Inferring causal linkages in longitudinal omics studies using econometric tools<br>*Gerard Bryan Gonzales, Wageningen University, Netherlands* | **57** |

| Tuesday, June 21 | | |
|---|---|---|
| **Time** | **Session** | **Abstract #** |
| **10:15 a.m. – 12 noon** | **Session 6. Plant Metabolomics**<br>*Session Chairs: Robert Hall and Carla Antonio* | *Multi Purpose 1* |
| 10:15 a.m. – 10:45 a.m. | **6.1 KEYNOTE**<br>HPTLC application to metabolomics as a supplementary tool for in-silica identification<br>*Young Hae Choi, Institute of Biology, Leiden University, Netherlands* | **418** |
| 10:45 a.m. – 11:05 a.m. | **6.2**<br>Combining Metabolomics and Phenomics approach to determinate horticultural plant stress response under different conditions<br>*Paolo Bonini, oloBion, Spain* | **235** |
| 11:05 a.m. – 11:20 a.m. | **6.3**<br>SlS5H silencing reveals specific pathogen-triggered salicylic acid metabolism in tomato<br>*Celia Payá, IBMCP, Spain* | **97** |
| 11:20 a.m. – 11:40 a.m. | **6.4**<br>Multi-Omics Analysis Provides Insights into the Acclimation of Plants to High-light Stress<br>*Gerd U. Balcke, Leibniz-Institute of Plant Biochemistry, Deutschland* | **284** |
| 11:40 a.m. – 11:55 a.m. | **6.5**<br>Mass spectrometry imaging allows plant metabolome changes in response to mycotoxin accumulation to be spatially resolved<br>*Laura Righetti, Food and Drug Department, University of Parma, Italy* | **135** |
| **12:20 p.m. – 1:20 p.m.** | **Sponsor Lunch Presentations** | |
| | **Bruker**<br>Expanding the Horizons of Metabolomics Research<br>*Ron M.A. Heeren, Maastricht University, Netherlands*<br>*Oscar Millet, CiC BioGUNE, Spain* | *Auditorium 1* |
| | **SCIEX**<br>Qualitative flexibility combined with quantitative power using the ZenoTOF 7600 system<br>*Thomas Hankemeier, Professor Of Analytical Bioscience, Leiden University*<br>*Sophie Ayciriex, Associate Professor, University Claude Bernard Lyon 1* | *Auditorium 2* |

***AWARD WINNERS**

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

***AWARD WINNERS**

| Tuesday, June 21 | | |
|---|---|---|
| **Time** | **Session** | **Abstract #** |
| **1:30 p.m. – 3 p.m.** | **Session 9. Technology Advancements I**<br>*Session Chairs: Leo Cheng and Guillermo Quintás* | *Multi Purpose 1* |
| 1:30 p.m. – 1:50 p.m. | **9.1**<br>Subcellular metabolomics – lessons learned from a compartment-specific metabolic investigation in a mouse model of Leigh syndrome<br>*Roan Louw, North-West University, South Africa* | **420** |
| 1:50 p.m. – 2:05 p.m. | **9.2**<br>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)<br>*Mariya Misheva, University Of Oxford, United Kingdom* | **203** |
| 2:05 p.m. – 2:25 p.m. | **9.3**<br>Stool metabolome of four NIST stool reference material<br>*Raquel Cumeras, Universitat Rovira i Virgili, Spain* | **115** |
| 2:25 p.m. – 2:40 p.m. | **9.4**<br>Development of a High-Coverage and Quantitative Metabolomics Assay for Targeted Analysis of Multiple Pathways<br>*Shuang Zhao, The Metabolomics Innovation Centre (TMIC), Canada* | **336** |
| 2:40 p.m. – 3 p.m. | **9.5**<br>Extending the Scope of 1H NMR Based Blood Metabolomics for the Analysis of Labile Antioxidants: Reduced and Oxidized Glutathione<br>*G. A. Nagana Gowda, Univesity Of Washington, United States* | **278** |
| **3:30 p.m. – 5 p.m.** | **Session 10. Lipidomics and Cardiovascular Diseases**<br>*Session Chairs: Jules Griffin and Stefania Noerman* | *Auditorium 1* |
| 3:30 p.m. – 3:50 p.m. | **10.1**<br>Lipidomic Latent Features Mediate Genetic Contributions to Coronary Heart Disease Risk: The Multi-Ethnic Study of Atherosclerosis (MESA)<br>*David Herrington, Wake Forest University School Of Medicine, United States* | **304** |
| 3:50 p.m. – 4:05 p.m. | **10.2**<br>Using OMICs to explore underlying pathways linking persistent organic pollutant exposures to cardiovascular disease in the Swedish Mammography Cohort<br>**Yingxiao YAN, Chalmers University of Technology, Sweden* | **77** |
| 4:05 p.m. – 4:25 p.m. | **10.3**<br>Lipidomics and flaxomics analysis reveals a novel role for fatty acid synthase in cholesterol and glycerolipid synthesis regulation in vivo.<br>*Mikhail Golovko, UND, United States* | **288** |
| 4:25 p.m. – 4:40 p.m. | **10.4**<br>Metabolomics and lipidomics at the top: Characterizing hypoxic responses of dwellers living permanently in La Rinconnada, the highest city of the world (5100m)<br>*Jean-Charles Martin, INRAE, France* | **185** |
| 4:40 p.m. – 5 p.m. | **10.5**<br>Targeted metabolomic profiles among genetically confirmed familial hypercholesterolemia, dyslipidemia without familial hypercholesterolemia and healthy controls.<br>*Teodoro Bottiglieri, Baylor Scott & White Research Institute, United States* | **364** |

***AWARD WINNERS**

| Tuesday, June 21 | | |
|---|---|---|
| **Time** | **Session** | **Abstract #** |
| **3:30 p.m. – 5 p.m.** | **Session 11. Vendor Session**<br>**(Presented by Platinum and Gold Sponsors)**<br>*Session Chair: Oscar Yanes* | *Auditorium 2* |
| 3:30 p.m. – 4:15 p.m. | **PLATINUM PRESENTERS –**<br>**SCIEX:** Jean-Baptiste Vincendet, Life Sciences Research Market Development, France<br>**Thermo Fisher Scientific:** Susan S. Bird, Sr. Manager, Metabolomics Marketing, USA<br>**Bruker:** Claire Cannet, Clinical Market Manager, Germany<br>**Agilent Technologies, Inc:** Genevieve Van de Bittner, R&D Researcher, USA | |
| 4:15 p.m. – 5:00 p.m. | **GOLD PRESENTERS –**<br>**LECO Corporation:** David E. Alonso, Applications Chemist, USA<br>**Metware Biotechnology:** Jeffrey Chu, General Manager, North America, USA<br>**Shimadzu Europa GmbH:** Emily Armitage, Research Scientist, UK<br>**Biocrates Life Sciences AG:** Alice Limonciel, Senior Scientist \| Data Interpretation, Austria | |
| **3:30 p.m. – 5 p.m.** | **Session 12. Plant and Environmental Applications I**<br>*Session Chairs: Maria Pilar Lopez Gresa and Gerhard Prinsloo* | *Multi Purpose 1* |
| 3:30 p.m. – 3:50 p.m. | **12.1**<br>Extending metabolome coverage through a multi-platform approach: the effect of low-dose polychlorinated biphenyls on pig metabolism<br>*Luca Narduzzi, University Of Granada, Spain* | **170** |
| 3:50 p.m. – 4:05 p.m. | **12.2**<br>Computational metabolomics tools reveal metabolic reconfigurations underlying the effects of biostimulant seaweed extracts on maize plants under drought stress conditions<br>*Morena Tinte, University Of Johannesburg, South Africa* | **181** |
| 4:05 p.m. – 4:25 p.m. | **12.3**<br>Imbibitional metabolite leakage in Linum usitatissimum L. seeds is shortened by plasma modification of the seed cuticle<br>*Rebecca Dauwe, Université de Picardie Jules Verne, France* | **125** |
| 4:25 p.m. – 4:40 p.m. | **12.4**<br>Leaf metabolomic changes of temperate and tropical seagrass species under future climate change<br>*Maria Jung, The University of Western Australia, Australia* | **118** |
| 4:40 p.m. – 5 p.m. | **12.5**<br>Development of Rapid Evaporative Ionisation Mass Spectrometry (REIMS) for in situ Metabolomics of Plants and Seeds<br>**Alice Flint, Queen's University Belfast, United Kingdom* | **266** |

***AWARD WINNERS**

| Wednesday, June 22 | | |
|---|---|---|
| **Time** | **Session** | **Abstract #** |
| **8:30 a.m. – 9:30 a.m.** | **Plenary Session 3**<br>Ultra-Resolution Plant Metabolomics: High Confidence Metabolite Identification and Spatial Analysis at the Cell Type and Organelle Level<br>*Asaph Aharoni, Weizmann Institute of Science, Israel* | *Auditorium 1* |
| **10:15 a.m. – 12 noon** | **Session 13. Cancer**<br>*Session Chairs: Margret Thorsteinsdottir and Laimdota Zizmare* | *Auditorium 1* |
| 10:15 a.m. – 10:45 a.m. | **13.1 SESSION KEYNOTE**<br>The metabolomic way for the screening of endometrial cancer<br>*Jacopo Troisi, Theoreo srl – spinoff company of the University of Salerno, Italy* | **112** |
| 10:45 a.m. – 11:05 a.m. | **13.2**<br>Longitudinal modelling reveals distinct changes in circulating metabolites and lipoprotein subfractions after breast cancer treatment<br>*Guro F. Giskeødegård, Norwegian University of Science and Technology, Norway* | **182** |
| 11:05 a.m. – 11:20 a.m. | **13.3**<br>Discovery and validation of a pre-diagnostic metabolic marker of glioma<br>*Sebastian Jonsson, Department of Chemistry, Umeå University, Sweden* | **196** |
| 11:20 a.m. – 11:40 a.m. | **13.4**<br>From features to function: Combining new metabolomics methods to study disease and treatment mechanisms in cancer cells<br>*James Mccullagh, University Of Oxford, United Kingdom* | **325** |
| 11:40 a.m. – 11:55 a.m. | **13.5**<br>Stable Isotope tracing uncovers global metabolic reprogramming and candidate cancer susceptibility pathways in Fanconi Anemia<br>*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**<br>*Session Chairs: Fabien Jourdan and Vinicius Veri* | *Auditorium 2* |
| 10:15 a.m. – 10:45 a.m. | **14.1 SESSION KEYNOTE**<br>GNPS Dashboard: collaborative exploration of mass spectrometry data in the web browser<br>*Mingxun Wang, UC San Diego, United States* | **237** |
| 10:45 a.m. – 11:05 a.m. | **14.2**<br>MZmine 3 – a tool from and for the mass spectrometry community<br>*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**<br>CloMet: A novel cloud-based platform that connects established metabolomics data repositories and data analysis platforms.<br>*Roger Mallol, La Salle – Universitat Ramon Llull, Spain* | **300** |
| 11:20 a.m. – 11:40 a.m. | **14.4**<br>RaMP 2.0 and MetaboSPAN: a public framework for extracting biological and chemical insight from metabolomic and multi-omic data<br>*Ewy Mathe, National Center For Advancing Translational Sciences, United States* | **262** |
| 11:40 a.m. – 11:55 a.m. | **14.5**<br>FORVM: a Knowledge Graph to decipher associations between metabolites and diseases<br>**Maxime Delmas, INRAE UMR 1331 ToxAlim, France* | **101** |

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| Wednesday, June 22 | | |
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| **Time** | **Session** | **Abstract #** |
| **10:15 a.m. – 12 noon** | **Session 15. Technology Advancements II**<br>*Session Chairs: Roy Goodacre and Dimitrios Damalas* | *Multi Purpose 1* |
| 10:15 a.m. – 10:45 a.m. | **15.1 KEYNOTE**<br>Next Gen Metabolomics Technologies: Deeper Coverage, Single Cell, Double Bond Pinpointing, Ion Mobility and Imaging<br>*Facundo Fernandez, Georgia Institute Of Technology, United States* | **389** |
| 10:45 a.m. – 11:05 a.m. | **15.2**<br>Breath analysis by secondary electrospray high-resolution mass spectrometry: An interoperability framework for multicentric studies and metabolic phenotyping<br>**Kapil Dev Singh, University of Basel, Switzerland* | **138** |
| 11:05 a.m. – 11:20 a.m. | **15.3**<br>A universal ion mobility calibration for interoperable collision cross section databases<br>*Anaïs George, Laboratoire COBRA, France* | **45** |
| 11:20 a.m. – 11:40 a.m. | **15.4**<br>Mapping the metabolome of living cells using Laser Desorption-Rapid Evaporative Ionization Mass Spectrometry (LD-REIMS)<br>*Stefania Maneta-Stavrakaki, Imperial College London, United Kingdom* | **322** |
| 11:40 a.m. – 11:55 a.m. | **15.5**<br>Ion Mobility Mass Spectrometry for the Characterization of Urolithin Glucuronides<br>*Maria Moran-Garrido, Centro de Metabolómica y Bioanálisis (CEMBIO), Facultad de Farmacia, Universidad San Pablo-CEU, CEU Universities, Spain* | **225** |
| **12:20 p.m. – 1:20 p.m.** | **Sponsor Lunch Presentations** | |
| | **Agilent**<br>Deciphering the Mechanisms of Immunometabolism in Eukaryotes and Drug Resistance in Bacteria using Extracellular Flux Analysis and 13C Stable-Isotope Tracing<br>*Dr. Gerald Larrouy-Maumus, Senior Lecturer, Imperial College London* | *Auditorium 1* |
| | **Thermo Fisher Scientific**<br>Crossing the Chasm in Metabolomics<br>*Maria Fedorova – Group Leader, TU Dresden; Julijana Ivanisevic – Faculty of Biology and Medicine, University of Lausanne; Oliver Fiehn – West Coast Metabolomics Center UC Davis Genome Center* | *Auditorium 2* |

| Wednesday, June 22 | | |
|---|---|---|
| **Time** | **Session** | **Abstract #** |
| **1:30 p.m. – 3 p.m.** | **Session 16. Lung and Respiratory Diseases**<br>*Session Chairs: Craig Wheelock and Julia Kuligowski* | *Auditorium 1* |
| 1:30 p.m. – 1:50 p.m. | **16.1**<br>MiR-342-3p and immune mediated metabolic signatures as drivers of long-term lung trajectories<br>*Sofina Begum, Brigham And Women's Hospital, Harvard Medical School, United States* | **296** |
| 1:50 p.m. – 2:05 p.m. | **16.2**<br>Non-Invasive Prediction of Oxidative Stress and Inflammation Markers in Children by Exhaled Breath Metabolites<br>*Amanda Gisler, University Children's Hospital Basel UKBB, University Of Basel, Switzerland, Switzerland* | **63** |
| 2:05 p.m. – 2:25 p.m. | **16.3**<br>GC-MS profiling of volatile metabolites produced by bacteria causing Ventilation-Associated Pneumonia<br>*Wojciech Filipiak, Dept of Pharmacodynamics and Molecular Pharmacology, Collegium Medicum UMK, Poland* | **306** |
| 2:25 p.m. – 2:40 p.m. | **16.4**<br>Benchtop Nuclear Magnetic Resonance-based metabolomic approach for the diagnosis of tuberculosis<br>*Jose Luis Izquierdo García, UCM, España* | **332** |
| 2:40 p.m. – 3 p.m. | **16.5**<br>Multi-omic landscape of squamous cell lung cancer<br>*Paul Stewart, Moffitt Cancer Center, United States* | **109** |
| **1:30 p.m. – 3 p.m.** | **Session 17. Plant and Environmental Applications II**<br>*Session Chairs: Ian Dubery and Antonio Granell* | *Auditorium 2* |
| 1:30 p.m. – 1:50 p.m. | **17.1**<br>Fingerprinting of tea varieties using a novel untargeted metabolomics workflow<br>*Daniel Hermanson, Thermo Fisher Scientific, United States* | **281** |
| 1:50 p.m. – 2:05 p.m. | **17.2**<br>1HNMR-based metabolomics analysis as a tool to identify antiviral compounds from unrelated plants<br>*Gerhard Prinsloo, University Of South Africa, South Africa* | **54** |
| 2:05 p.m. – 2:25 p.m. | **17.3**<br>Utility of Metabolomics to Support Read-Across and Category Justification for UVCB substances in REACH<br>*Hennicke Kamp, Basf Metabolome Solutions Gmbh, Germany* | **299** |
| 2:25 p.m. – 2:40 p.m. | **17.4**<br>Gut metabolomics after the exposure to diclofenac and selenium supplementation<br>*Gema Moro, University Of Huelva, Spain* | **133** |
| 2:40 p.m. – 3 p.m. | **17.5**<br>Coupling growth of Pseudomonas putida to a synthetic fluorination metabolism<br>*Corey Griffith, Luxembourg Centre for Systems Biomedicine, Luxembourg* | **187** |

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

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## Wednesday, June 22

| Time | Session | Abstract # |
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| **3:30 p.m. – 5 p.m.** | **Session 20. Met ID II**<br>*Session Chairs: Alvaro Fernandez Ochoa and Justin JJ Van der Hooft* | *Auditorium 2* |
| 3:30 p.m. – 3:50 p.m. | **20.1**<br>Improving reliability of small molecule identification using spectral entropy and retention time prediction<br>*Sajjan Mehta, oloBion, Spain* | **189** |
| 3:50 p.m. – 4:05 p.m. | **20.2**<br>CPExtract, a novel software tool for the comprehensive detection of tracer-derived metabolites in high resolution mass spectrometry data<br>*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**<br>Ion Identity Molecular Networking for Mass Spectrometry-based Metabolomics<br>*Robin Schmid, Skaggs School of Pharmacy, University of California San Diego, United States* | **239** |
| 4:25 p.m. – 4:40 p.m. | **20.4**<br>Multi-network integration to analyze non-targeted LC-MS metabolomics data from Caenorhabditis elegans<br>*Liesa Salzer, Helmholtz Zentrum Muenchen, Germany* | **51** |
| 4:40 p.m. – 5 p.m. | **20.5**<br>CMM 4.0: improving the metabolite annotation using RT and CCS prediction<br>*Alberto Gil-de-la-fuente, CEU-San Pablo University, Spain* | **234** |
| **3:30 p.m. – 5 p.m.** | **Session 21. Metabolic Diseases**<br>*Session Chairs: Rachel Kelly and Natasa Giallourou* | *Multi Purpose 1* |
| 3:30 p.m. – 3:50 p.m. | **21.1**<br>Lipidomic profile of white adipose tissue associated with obesity and insulin resistance in pregnant women with previous bariatric surgery<br>**Susana Alejandra Palma Duran, The Francis Crick Institute, United Kingdom* | **337** |
| 3:50 p.m. – 4:05 p.m. | **21.2**<br>UHPLC-MS/MS-based Metabolomics reveals differences on Extracellular Vesicles secreted by obese hepatocytes, and their effects on adipocyte metabolism<br>*Maria Azparren-Angulo, Cicbiogune, Spain* | **154** |
| 4:05 p.m. – 4:25 p.m. | **21.3**<br>Low carbohydrate high fat diet improves composition of the circulating lipids in people with type 2 diabetes<br>*Kajetan Trošt, University of Copenhagen, Denmark* | **92** |
| 4:25 p.m. – 4:40 p.m. | **21.4**<br>Plasma metabolic profile of subclinical atherosclerosis in South-East Asians.<br>*Nilanjana Sadhu, Nanyang Technological University Lee Kong Chian School of Medicine, Singapore* | **193** |
| 4:40 p.m. – 5 p.m. | **21.5**<br>NAD+ – an old cofactor with new tricks<br>*Sofia Moco, VU Amsterdam, Netherlands* | **312** |

## METABOLOMICS IN HEALTH AND DISEASE
## PLANTS, FOOD, ENVIRONMENT AND MICROBES

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| Thursday, June 23 | | |
|---|---|---|
| **Time** | **Session** | **Abstract #** |
| **8:30 a.m. – 10:15 a.m.** | **Session 22. Microbiome and Gastrointestinal Function**<br>*Session Chairs: Daniel Raftery and Maria Eugenia Monge* | *Auditorium 1* |
| 8:30 a.m. – 9:00 a.m. | **22.1 SESSION KEYNOTE**<br>Spatial-, temporal- and inter-person variation of metabolites across the upper and lower human gastrointestinal tract.<br>*Oliver Fiehn, UC Davis, United States* | **253** |
| 9:00 a.m. – 9:20 a.m. | **22.2**<br>Quantitative Sensitive CHEmoselective Metabolomics Analysis (Quant-SCHEMA) – Detailed investigation of microbiome metabolism<br>*Daniel Globisch, Uppsala University, Sweden* | **228** |
| 9:20 a.m. – 9:35 a.m. | **22.3**<br>Chemical exposures are associated with altered microbiome and secondary bile acid pathways in obesity and insulin resistance<br>*Partho Sarathi Sen, Turku Bioscience, University Of Turku, Finland* | **186** |
| 9:35 a.m. – 9:55 a.m. | **22.4**<br>Gut microbiome-linked metabolites in the pathobiology of depression and anxiety – a role for bile acids<br>*Rima Kaddurah-Daouk, Duke University Medical Center, United States* | **359** |
| 9:55 a.m. – 10:10 a.m. | **22.5**<br>Metabolome Alterations in a Mouse Model Support Microbiome-Metabolite Interactions in a Cohort of Children With Cow's Milk Allergy<br>*Ellen De Paepe, Ghent University, Belgium* | **165** |
| **8:30 a.m. – 10:15 a.m.** | **Session 23. Natural Products**<br>*Session Chairs: Lloyd Sumner and Maria Garcia Altares* | *Auditorium 2* |
| 8:30 a.m. – 9:00 a.m. | **23.1 SESSION KEYNOTE**<br>Helichrysum umbraculigerum: A new plant system for cannabinoid biochemistry<br>*Paula Berman, Weizmann Institute of Science, Israel* | **315** |
| 9:00 a.m. – 9:20 a.m. | **23.2**<br>Unraveling 100 plant glycosyltransferases with 600 Natural compounds: results of a combinatorial screen<br>**Elys Rodriguez, Fiehn Lab, United States* | **257** |
| 9:20 a.m. – 9:35 a.m. | **23.3**<br>Deciphering the Complex Chemical Space and Biosynthetic Routes of Steroidal Saponins in Monocotyledonous Plants<br>*Adam Jozwiak, Weizmann Institute of Science, Israel* | **318** |
| 9:35 a.m. – 9:55 a.m. | **23.4**<br>Identification of natural products as potential plant-derived herbicides through metabolomics<br>*Monica Scognamiglio, University Of Campania "Luigi Vanvitelli", DiSTABiF, Italy* | **316** |
| 9:55 a.m. – 10:10 a.m. | **23.5**<br>Exploiting metabolic diversity in Nicotiana for intragenic production of squalene<br>*Margit Drapal, Royal Holloway University Of London, United Kingdom* | **177** |

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| Thursday, June 23 | | |
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| **Time** | **Session** | **Abstract #** |
| **8:30 a.m. – 10:15 a.m.** | **Session 24. Analytical Methods in Lipidomics**<br>*Session Chairs: Matej Oresic and Susana Palma* | *Multi Purpose 1* |
| 8:30 a.m. – 9:00 a.m. | **24.1 KEYNOTE**<br>Lipidomics and epilipidomics signature of human obesity and insulin resistance<br>*Maria Fedorova, Technical University Dresden, Germany* | **454** |
| 9:00 a.m. – 9:20 a.m. | **24.2**<br>Metabolic profiling of octadecanoid oxylipins using chiral supercritical fluid chromatography coupled to tandem mass spectrometry<br>*Craig Wheelock, Karolinska Institute, Sweden* | **292** |
| 9:20 a.m. – 9:35 a.m. | **24.3**<br>High-throughput Plasma Lipidomics using Ion-mobility enhanced DDA and DIA Mass Spectrometry (DDA-PASEF/diaPASEF)<br>*Premy Shanthamoorthy, University of Toronto, Canada* | **66** |
| 9:35 a.m. – 9:55 a.m. | **24.4**<br>Complete structure elucidation of lipids by electron activated dissociation mass spectrometry<br>*Takashi Baba, Sciex, Canada* | **134** |
| 9:55 a.m. – 10:10 a.m. | **24.5**<br>Ultra-high throughput metabolomics and lipidomics: Results from the first 5,000 samples<br>**Zach Rabow, UC Davis, United States* | **350** |
| **11:30 a.m. – 1 p.m.** | **Plenary Session 4 and Awards / Closing**<br>Analytical Challenges in Untargeted Metabolomics Workflow<br>*Coral Barbas, Universidad San Pablo CEU, Spain* | *Auditorium 1* |
| **1 p.m.** | **Boxed Lunch to Go** | |