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** 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 Debik, 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**

***AWARD WINNERS**

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

Tuesday, June 21		
Time	**Session**	**Abstract #**
10:15 a.m. – 12 noon	**Session 6. Plant Metabolomics** *Session Chairs: Robert Hall and Carla Antonio*	*Multi Purpose 1*
10:15 a.m. – 10:45 a.m.	**6.1 KEYNOTE** HPTLC application to metabolomics as a supplementary tool for in-silica identification *Young Hae Choi, Institute of Biology, Leiden University, Netherlands*	**418**
10:45 a.m. – 11:05 a.m.	**6.2** Combining Metabolomics and Phenomics approach to determinate horticultural plant stress response under different conditions *Paolo Bonini, oloBion, Spain*	**235**
11:05 a.m. – 11:20 a.m.	**6.3** SlS5H silencing reveals specific pathogen-triggered salicylic acid metabolism in tomato *Celia Payá, IBMCP, Spain*	**97**
11:20 a.m. – 11:40 a.m.	**6.4** Multi-Omics Analysis Provides Insights into the Acclimation of Plants to High-light Stress *Gerd U. Balcke, Leibniz-Institute of Plant Biochemistry, Deutschland*	**284**
11:40 a.m. – 11:55 a.m.	**6.5** Mass spectrometry imaging allows plant metabolome changes in response to mycotoxin accumulation to be spatially resolved *Laura Righetti, Food and Drug Department, University of Parma, Italy*	**135**
12:20 p.m. – 1:20 p.m.	**Sponsor Lunch Presentations**	
	Bruker Title TBD *Presenter TBD*	*Auditorium 1*
	SCIEX Qualitative flexibility combined with quantitative power using the ZenoTOF 7600 system *Jean-Baptiste Vincendet, Sr Market Development Manager, SCIEX*	*Auditorium 2*

***AWARD WINNERS**

Tuesday, June 21		
Time	**Session**	**Abstract #**
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** Metabolomic 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-Rodríguez, 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**

***AWARD WINNERS**

Tuesday, June 21		
Time	**Session**	**Abstract #**
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 1H NMR Based Blood Metabolomics for the Analysis of Labile Antioxidants: Reduced and Oxidized Glutathione *G. A. Nagana Gowda, Univesity 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**

***AWARD WINNERS**

Tuesday, June 21		
Time	**Session**	**Abstract #**
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:** Claire Cannet, Clinical Market Manager, Germany **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 | Data Interpretation, Austria	
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** Biostimulant effects of Chaetomium globosum and Minimedusa polyspora culture filtrates on Cichorium intybus plant: growth performance and metabolomic traits *Elisa Brasili, Dept. of Environmental Biology, Sapienza University of Rome, Italy*	**287**
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**

***AWARD WINNERS**

Wednesday, June 22		
Time	**Session**	**Abstract #**
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: Margret Thorsteinsdottir 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**

***AWARD WINNERS**

Wednesday, June 22		
Time	**Session**	**Abstract #**
10:15 a.m. – 12 noon	**Session 15. Technology Advancements II** *Session Chairs: Roy Goodacre and Dimitrios Damalas*	*Multi Purpose 1*
10:15 a.m. – 10:45 a.m.	**15.1 KEYNOTE** Next Gen Metabolomics Technologies: Deeper Coverage, Single Cell, Double Bond Pinpointing, Ion Mobility and Imaging *Facundo Fernandez, Georgia Institute Of Technology, United States*	**389**
10:45 a.m. – 11:05 a.m.	**15.2** Breath analysis by secondary electrospray high-resolution mass spectrometry: An interoperability framework for multicentric studies and metabolic phenotyping **Kapil Dev Singh, University of Basel, Switzerland*	**138**
11:05 a.m. – 11:20 a.m.	**15.3** A universal ion mobility calibration for interoperable collision cross section databases *Anaïs George, Laboratoire COBRA, France*	**45**
11:20 a.m. – 11:40 a.m.	**15.4** Mapping the metabolome of living cells using Laser Desorption-Rapid Evaporative Ionization Mass Spectrometry (LD-REIMS) *Stefania Maneta-Stavrakaki, Imperial College London, United Kingdom*	**322**
11:40 a.m. – 11:55 a.m.	**15.5** Ion Mobility Mass Spectrometry for the Characterization of Urolithin Glucuronides *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 Deciphering the Mechanisms of Immunometabolism in Eukaryotes and Drug Resistance in Bacteria using Extracellular Flux Analysis and 13C Stable-Isotope Tracing *Dr. Gerald Larrouy-Maumus, Senior Lecturer, Imperial College London*	*Auditorium 1*
	Thermo Fisher Scientific Crossing the Chasm in Metabolomics *Susan Bird, Sr. Manager, Metabolomics Vertical Marketing Group, Thermo Fisher Scientific*	*Auditorium 2*

Wednesday, June 22		
Time	**Session**	**Abstract #**
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** Fingerprinting of tea varieties using a novel untargeted metabolomics workflow *Daniel Hermanson, Thermo Fisher Scientific, United States*	**281**
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**

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

***AWARD WINNERS**

Wednesday, June 22		
Time	**Session**	**Abstract #**
3:30 p.m. – 5 p.m.	**Session 20. Met ID II** *Session Chairs: Alvaro Fernandez Ochoa and Justin JJ Van der Hooft*	*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**

METABOLOMICS IN HEALTH AND DISEASE
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***AWARD WINNERS**

Thursday, June 23		
Time	**Session**	**Abstract #**
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** Spatial-, 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: Lloyd Sumner 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**

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