22nd Annual Conference of the Metabolomics Society

METABOLOMICS 2026

BUENOS AIRES ARGENTINA | JUNE 21-24

Pre-Conference Workshops

Sunday, June 21 8:15 a.m. – 10:15 a.m.

W1: Cross-repository discoverability, harmonization, and analysis of public metabolomics data with MetabolomicsHub

Presenters

- **Thomas Payne,** EMBL-EBI
- **Yasin El Abiead,** University of Natural Resources and Life Sciences Vienna
- **Eoin Fahy,** University of California San Diego
- **Callum Martin,** EMBL-EBI
- **Juan Antonio Vizcaíno,** EMBL-EBI

Description

The growing availability of public metabolomics data offers unprecedented opportunities for reuse, integration and large-scale analyses. However, meaningful exploitation of these data remains limited by fragmentation across repositories and heterogeneity in metadata, formats, identifiers and access mechanisms.

Under the MetabolomicsHub initiative (https://metabolomicshub.org) - spanning MetaboLights (European Bioinformatics Institute, UK), Metabolomics Workbench and GNPS/MassIVE (University of California San Diego, USA) - coordinated efforts in shared infrastructure, data standardization and metadata harmonization have started to address these challenges and lay the groundwork towards cross-repository discoverability, harmonization and generalization of (re)analysis of public metabolomics data. The overall aim of MetabolomicsHub is to standardize and generalize open and FAIR data practices in line with efforts in other fields.

This workshop will explore current challenges and key developments and resources for cross-repository discoverability, harmonization and integrated analysis of public metabolomics data. Through short presentations, live demonstrations and interactive discussion, participants will learn how datasets can be discovered across repositories, how metadata can be aligned, and how harmonized access enables integrative analyses across studies and omics layers. Emphasis will be placed on real-world examples, community standards and emerging tools and workflows, including panReDU, structureMASST, RefMet, and the MetabolomicsHub Common Data Model and Data Portal.

Workshop Objectives

- Highlight challenges and opportunities in cross-repository discoverability, harmonization and analysis of public metabolomics data.
- Demonstrate key developments, resources and real-world use cases that span data discovery, harmonized access and integrative analysis across studies and omics layers.
- Promote community adoption of best practices and encourage contribution to shared standards, infrastructure and outreach efforts.

Learning Outcomes

- Understand the current landscape of metabolomics data repositories and the value of public FAIR metabolomics data.
- Identify key initiatives, tools and workflows that enable cross-repository discoverability, harmonization and analysis of public metabolomics data through real-world examples.
- Recognize and engage best practices and community efforts aimed to support FAIR metabolomics data.

Updated May 29

Sunday, June 21 8:15 a.m. – 10:15 a.m.

W2: Demystifying Stable Isotope Labelling Metabolomics

Presenters

- **James MacRae,** The Francis Crick Institute, UK
- **Bart Ghesquiere,** KU Leuven, Belgium
- **Shauni Loopmans** KU Leuven, Belgium
- **David De Souza,** Metabolomics Australia, The Bio21 Institute, Australia

Description

Metabolite profiling and targeted metabolomics approaches are now routinely applied by researchers wanting to understand the physiology of their cell, tissue, organism, or biofluid of choice.

One of the largest challenges faced by metabolomics researchers in any study is relating changes in identified metabolites to their metabolic roles. Understanding this relationship is critical for understanding metabolic mechanisms in that biosystem.

Stable isotope labelling has rapidly emerged as a powerful tool in unravelling the precise structure and activity of metabolic pathways and how these influence/are caused by the physiological state of the biosystem. These techniques can reveal subtle alterations in metabolic activity that would not be possible with unlabeled approaches. This depth of information can provide valuable insight into the mechanisms that underlie various physiological conditions and aberrant processes, including infection and disease.

This workshop will show how metabolic labelling studies are readily approachable and easily interpretable when performed correctly. Covering in vitro, in vivo, and imaging approaches, we will show you how to design, run, and analyse stable isotope labelling experiments, and explain how these simple workflows are often sufficient for significant biological insight.

New for 2026! A little look at lipids

Workshop Objectives

- Know how to design a labelling project, including essentials to consider and potential pitfalls.
- Know the basics of analysis of labelling data, including awareness of some of the available LC-MS and GC-MS software.
- Understand how to interpret data, including the importance of mass isotope distributions.

Learning Outcomes

- That stable isotope labelling projects are easy to design, perform, and interpret.
- That labelling experiments can bring intricate detail to many metabolomics projects, whether untargeted or targeted, or polar or lipid-focused.
- Key principles for in vitro and in vivo labelling studies, combining labelling with mass spectrometry imaging, and multi-isotope approaches.

W3: LC-MS Data Processing with mzmine

****Hands-On Session – Laptop Required**

Presenters

- **Federico Brigante,** IOCB Prague
- **Katerina Kucerova,** IOCB Prague

Description

LC-MS is arguably the most popular analytical technique for metabolomics analysis, and mzmine is one of the most popular software for LC-MS data processing and annotation. This hands-on workshop will provide an overview of LC-MS data Processing in mzmine using an example dataset. The workshop will cover:

- Introduction to LC-MS metabolomics and exploration of raw data with mzmine.
- LC-MS metabolomics data processing (e.g., feature detection) with mzmine.
- Overview of downstream data analysis tools in mzmine (e.g., molecular networking, statistical analysis).

Ample time will be dedicated to Q&A so that specific problems and individual use cases can also be discussed.

Workshop Objectives

- Introducing untargeted LC-MS/MS data processing in mzmine.
- Feature detection, compound annotation, and molecular networking in mzmine.
- Exporting results from mzmine to interface other tools like SIRIUS and GNPS.

Learning Outcomes

- How to create the first batch file using the mzwizard.
- Inspect intermediate and final processing outputs (i.e., feature tables).
- Use downstream analysis tools in mzmine (statistics, molecular networking).

Sunday, June 21 10:30 a.m. – 12:30 p.m.

W4: Metabolomics and AI Approaches for Precision Health and Precision Medicine

Presenters

- **Rima Kaddurah-Daouk,** Duke University
- **David Wishart,** University of Alberta
- **Jennifer Kirwan,** University of Veterinary Medicine, Vienna | Berlin Institute of Health at Charité Universitätsmedizin
- **Susan Sumner,** UNC Chapel Hill
- **Matej Oresic**, Örebro University & University of Turku
- **Tuulia Hyötyläinen**, Örebro University
- Invited team members from workshop ***W1: Cross-repository discoverability, harmonization, and analysis of public metabolomics data with MetabolomicsHub*** for a cross talk between the 2 workshops

Description

Precision medicine and precision health differ in both timing and focus. Precision medicine is largely reactive: it seeks the right drug for the right person at the right time, applying genomic insights to diagnose disease, select therapies, and tailor treatment once illness has emerged. Precision health, by contrast, is proactive and preventative. It emphasizes maintaining wellness before disease develops, using metabolomics, exposomics, diet, lifestyle, and environmental measures to understand an individual's real-time biochemical state. Where precision medicine treats genetic risk and clinical symptoms, precision health monitors dynamic physiology and modifiable exposures to reduce risk, delay disease, and promote long-term health. We will be sharing how metabolomics, lipidomics, exposomics, foodomics, metagenomics and genomics data combined with digital data and AI tools can reshape health care in the future and define a key role for our metabolomics community in proactive health.

Workshop Objectives

- Learn about metabolomics applications in precision medicine.
- Learn about complimentary approaches where metabolomics and digital data can be used synergistically and with AI tools to enable proactive health.
- Learn about interconnected influences of exposome, diet, gut microbiome and genome on human health and modifiable factors.

Learning Outcomes

- Appreciate the power of metabolomics in highlighting influences of exposome, diet, gut microbiome and genome on human health.
- Learn about changes in health in real time and approaches to monitor such changes.
- Develop approaches leveraging modifiable factors for sustenance of health.

W5: From Unknowns to Structures: Introducing CHESS-Hub and Mapping Community Needs in Metabolite Identification

Presenters

- **Joanna Godzien,** Medical University of Bialystok
- **Jia Li,** Imperial College London
- **Anisha Wijeyesekera,** University of Reading
- **Coral Barbas**, Universidad San Pablo CEU

Description

Accurate metabolite identification remains a central challenge in metabolomics, limiting biological interpretation, biomarker discovery, and translation into clinical and industrial applications. Despite major advances in analytical instrumentation and computational tools, chemical structural elucidation of unknown metabolites is still fragmented across disciplines, laboratories, and methodologies.

This workshop introduces CHESS-Hub (CHEmical Structural Solutions for metabolites), a newly established international initiative aiming to advance chemical structural elucidation through collaboration, knowledge exchange, and training. The session will present CHESS-Hub's mission, motivations, and strategic vision.

A central component of the workshop will be an interactive community survey and discussion to identify key bottlenecks, unmet needs, and expectations for metabolite identification across diverse application areas. The collected feedback will directly inform future CHESS-Hub activities and strategies, ensuring they align with and best serve the community's real needs. This workshop is intended as an open forum to engage researchers at all career stages and foster collective progress toward more robust, transparent, and efficient structural elucidation workflows in metabolomics.

Workshop Objectives

- Introduce the CHESS-Hub initiative, its mission, structure, and planned activities to the global metabolomics community.
- Identify key challenges, unmet needs, and expectations related to metabolite identification through structured community feedback.
- Foster engagement and future collaboration between researchers across disciplines, career stages, and sectors.

Learning Outcomes

- Understand current challenges and emerging solutions in chemical structural elucidation for metabolite identification.
- Become familiar with the goals, resources, and opportunities offered by CHESS-Hub.
- Gain insight into community-driven strategies for improving metabolite identification workflows.

W6: MetaboApps in GNPS2: Hands-on Drug, Food, and Microbial Readouts with FBmn-stats for Untargeted Metabolomics LC-MS/MS-based

****Hands-On Session – Laptop Required**

Presenters

- **Lurian Caetano David**, Laboratory of Methods of Extraction and Separation, Federal University of Goias
- **Luís Feitosa**, Computational Chemical Biology Laboratory (CCBL), University of São Paulo
- **Prof. Ricardo Roberto da Silva**, Computational Chemical Biology Laboratory, University of São Paulo

Description

An important methodology that connects Global Natural Products Social Molecular Networking (GNPS) and mass spectrometry (MS) data processing tools is the feature-based molecular network (FBMN). Within the GNPS2 platform, MetaboApps provides a suite of downstream analysis tools that leverage FBMN outputs to facilitate biological interpretation of untargeted LC-MS/MS data. Drug and Food readouts are tools in this broader MetaboApps collection; each has its own library and is built from curated MS/MS spectra of foods and drugs. Drug readouts support the empirical annotation of drugs, their metabolites, and analogs, along with standardized data on their pharmacological properties. Food readouts apply a similar approach to food-derived compounds to estimate dietary intake composition. The Collaborative Microbial Metabolite Center (CMMC) Dashboard enables interactive exploration of enrichment results derived from the CMMC knowledgebase (CMMC-kb), supporting interpretation of microbial origins, metabolite sources, biological activity, and associated metadata. For enhanced statistical analysis of MS data matched to available metadata, FBmn-stats provides statistical techniques fitted for working with FBMN outputs.

Therefore, this workshop will present these resources within an integrated, explanatory, and hands-on format. Laptop use is recommended but optional, and participants will gain practical experience applying these workflows to analyze and interpret their own LC-MS/MS metabolomics datasets. Within the GNPS2 platform, MetaboApps provides a suite of downstream analysis tools that leverage FBMN outputs to facilitate biological interpretation of untargeted LC-MS/MS data. Drug and Food readouts are tools in this broader MetaboApps collection; each has its own library and is built from curated MS/MS spectra of foods and drugs. Drug readouts support the empirical annotation of drugs, their metabolites, and analogs, along with standardized data on their pharmacological properties. Food readouts apply a similar approach to food-derived compounds to estimate dietary intake composition. The Collaborative Microbial Metabolite Center (CMMC) Dashboard enables interactive exploration of enrichment results derived from the CMMC knowledgebase (CMMC-kb), supporting interpretation of microbial origins, metabolite sources, biological activity, and associated metadata.

For enhanced statistical analysis of MS data matched to available metadata, FBmn-stats provides statistical techniques fitted for working with FBMN outputs. Therefore, this workshop will present these resources within an integrated, explanatory, and hands-on format. Laptop use is recommended but optional, and participants will gain practical experience applying these workflows to analyze and interpret their own LC-MS/MS metabolomics datasets.

Workshop Objectives

- Introduce Drug and Food readout workflows for LC-MS/MS metabolomics data.
- Demonstrate enrichment analysis and interpretation using the CMMC dashboard.
- Guide participants through statistical analysis and validation of FBMN outputs using FBmn-stats.

Learning Outcomes

- Understand the operation of the tools, considering which data is being leveraged, and how to properly assess and validate the output acquired.
- Be able to upload and analyze metabolomics data through the apps for their own research.

W7: EMN Professional Career Development Workshop – Navigating Diverse Career Paths

Presenters

- **Alice Limonciel,** Bruker
- **Bart Ghesquiere,** VIB - KU Leuven
- **Fidele Tugizimana,** University of Johannesburg & Omnia Group Ltd
- **Monica Cala Molina,** Universidad de Los Andes
- **Rima Kaddurah-Daouk,** Duke University
- **Susan Bird,** Thermo Fisher Scientific
- **EMN Members**

Description

Following two successful editions of EMN career development workshop, EMN is back with a new workshop on navigating diverse career paths, a particularly timely topic as the landscape of career opportunities in science is evolving. This EMN workshop is designed for participants from different scientific backgrounds and career stages who are curious and attracted by the possibility of navigating diverse career paths. To help ECRs understand today's changing career landscape and give them practical guidance to explore and pursue different professional options, the workshop will be divided into three sections. Section 1, "Mapping the career landscape", will equip ECRs with a comprehensive understanding of career possibilities, revealing what each path offers and the trade-offs to consider. Section 2, "Building your career path: from skills to strategy", will focus on equipping ECRs with practical tools to navigate diverse career paths. The session will address how to recognise when a career transition may be timely, assess and translate skills across sectors, and strategically build networks to identify new opportunities. Finally, an open discussion (Section 3) between the audience, EMN committee members, and selected panelists will be held to provide a direct interaction with experts who have experienced and combined different career paths.

Workshop Objectives

Section 1: Mapping the career landscape

- Introduce career opportunities in metabolomics and related scientific fields.
- Map the landscape of career possibilities within and beyond traditional research roles.

Section 2: Building your career path: from skills to strategy

- Discuss key moments and indicators for shifting career paths
- Highlight the importance of developing and maintaining your network to find opportunities.

Section 3: Interactive panel and networking

- Connect participants with professionals who have navigated diverse career trajectories.
- Facilitate dialogue and networking that encourage participants to explore different career paths.

Learning Outcomes

- Identify the career landscape in metabolomics within and beyond academia and industry
- Develop strategies to evaluate and navigate your career path by leveraging your strengths, transferable skills, and professional networks
- Engage in an interactive discussion with a panel of experts, gaining insight into real-world career trajectories, including successes, struggles, and practical advice for navigating career paths

Sunday, June 21 1:30 p.m. – 3:30 p.m.

W8: The current state and future requirements for the use of Quality Control (QC) in untargeted metabolomics as defined by mQACC

Presenters

- **Victor Gonzalez-Ruiz**, CEMBIO, Universidad CEU-San Pablo, CEU Universities, Spain
- **Dajana Vuckovic**, Concordia University, Canada
- **Leo Cheng**, Corewell Health, United States
- **Jennifer Kirwan**, Veterinary Medical University of Vienna, Austria
- **Mariana Santos**, Medical Research Council (MRC) Laboratory of Medical Sciences (LMS), UK
- **Julia Kuligowski**, Health Research Institute La Fe, Spain

Description

There is a critical need to standardize and implement QA and QC practices in untargeted metabolomics to ensure high quality data generation, analysis and reporting of data quality. The metabolomics Quality Assurance and quality Control Consortium (mQACC) was established in 2017 and currently has over 140 international members operating across different working groups. It aims to develop, disseminate and harmonize best practices in untargeted metabolomics covering multiple analytical platforms. In this educational workshop, mQACC members will highlight the need for robust quality control in all untargeted metabolomics studies, present case studies illustrating QC sample types and their use across different analytical platforms (LC-MS, GC-MS, NMR spectroscopy) and conclude with a question-and-answer session to address audience questions. Finally, avenues for further engagement with mQACC will be presented.

Workshop Objectives

- To educate new adopters of untargeted metabolomics to the quality control (QC) principles and requirements.
- To disseminate best practices for quality control for different analytical platforms.
- To increase awareness of mQACC in South America and develop a strong network between South American metabolomics community and mQACC.

Learning Outcomes

- Attendees will learn best QC practices for untargeted metabolomics using LC-MS, GC-MS and NMR including best reporting practices.
- Attendees will be able to identify how to participate in mQACC, including mechanisms to contribute to the best practices community engagement efforts.

W9: From Metabolic Profiles to Biological Insights: An Introduction to MetExplore 3

Presenters

- **Dr. Ludovic Cottret,** NRAE, France
- **Dr. Fabien Jourdan,** INRAE, France
- **Pr. Timothy Ebbels,** Imperial College, UK

Description

Interpretation of metabolomics data is strengthened when metabolites are examined in the context of the network of metabolic reactions that produces and consumes them. MetExplore 3 is a web-server that couples curated genome-scale metabolic network with intuitive visualisation and statistical tools, allowing users to map experimental datasets, extract condition-specific subnetworks, and compute pathway enrichment—all without writing code.

In this workshop, we will first provide a concise overview of the challenges and concepts of omics-driven network analysis (1h30). Participants will learn how metabolic reconstructions are made, what are the requirements to map metabolomics data onto metabolic networks, what are the recommendations to compute pathway enrichment analysis and how metabolic network visualisation can help the interpretation of metabolomics data.

The second part is a live demo (1 h) in which participants will learn how to:

- Explore and query metabolic networks.
- Upload a metabolomics dataset to MetExplore 3.
- Perform a mapping and apply pathway enrichment.
- Generate, share an interactive sub-network, and export publication-ready figures.

All example files, step-by-step tutorials and the complete documentation will be hosted online, so participants can reproduce the demo on their own computers later.

Workshop Objectives

- Conceptual grounding – 40 min lecture on metabolic networks and omics integration.
- Hands-on proficiency – step-by-step guide through a full MetExplore 3 workflow.
- Independent use – online resources (docs, tutorials, talks) to enable users to use the site independently
- Feedback loop – collect user feedback for the next MetExplore 3 releases.

Learning Outcomes

- Understand why network-based analysis adds value to metabolomics data interpretation.
- Map metabolomics data, explore and visualise metabolic networks.
- Calculate pathway enrichment following metabolomics best practices.
- Export figures/tables suitable for publications.
- Locate resources for advanced analyses.

Sunday, June 21 1:30 p.m. – 3:30 p.m.

W10: Multisegment Injection-Capillary Electrophoresis-Mass Spectrometry: A High-throughput Platform for Large-scale Metabolomic Studies

**Hands-On Session – Laptop Required

Presenters

- **Philip Britz-Mckibbin,** McMaster University
- **Mariana Buitrago,** McMaster University

Description

Large-scale metabolomic studies remain hampered by low sample throughput, high operating costs, and inter-batch effects when using high efficiency separations coupled to electrospray ionization-mass spectrometry. This barrier is particularly significant in resource-limited settings where scalable, sustainable, and cost-effective technologies for population level studies in metabolomics are needed. This workshop will outline progress made in developing multisegment injection-capillary electrophoresis-mass spectrometry (MSI-CE-MS) as a multiplexed microseparation platform for untargeted analysis of polar/ionic metabolites in complex biological samples. We will present our recent efforts in implementing a standardized data workflow for metabolomics in large cohort studies, including software tools for automated data pre-processing and reliable peak picking in spite of large migration time variability. We anticipate that this workshop will provide researchers key insights into successful translation of MSI-CE-MS technology into their laboratory that will increase overall productivity at incremental costs.

Workshop Objectives

- To appreciate the historic barriers of adopting CE-MS in metabolomics.
- To understand principles of multiplexed separations in MSI-CE-MS for high-throughput metabolomics.
- To familiarize with automated data processing in metabolomics using a new software tool for MSI-CE-MS.

Learning Outcomes

- To appreciate the major technical challenges in conducting large-scale metabolomic studies.
- To understand the principles of multiplexed electrophoretic separations to realize high throughput metabolomic analyses.
- To familiarize with automated data processing in metabolomics using a new software tool developed for MSI-CE-MS.