METABOLOMICS
OSAKA, JAPAN
JUNE 16-20 2024

# Pre-Conference Workshops

## Sunday, June 16 12:00 p.m. – 2:00 p.m.

## W1: Nutritional Metabolomics - Biomarkers of Dietary Intake and Exposure

### Presenters

- **Daniel Raftery**, University of Washington
- **Oliver Fiehn**, University of California, Davis
- **Clary Clish**, Broad Institute of MIT and Harvard
- **Catalina Cuparencu**, University of Copenhagen
- **Steven Watkins**, Periodic Food Table Initiative
- **Lorraine Brennan**, University College Dublin
- **David Wishart**, University of Alberta

### Description

Adherence to healthy dietary patterns is important for reducing the risk of incidence of a variety of chronic diseases including obesity, diabetes, cardiovascular disease, and cancer. However, accurately assessing diet in free-living individuals remains a challenging aspect of nutrition research and thus there is a critical need to expand efforts to discover and validate objective biomarkers of dietary intake and food exposures. The objective of this workshop is to discuss approaches to using metabolomics to profile food specific metabolites and to discover biomarkers in clinical studies that can be used to evaluate health risk and ultimately affect dietary guidelines.

The workshop will be structured with a series of short introductory presentations to highlight past and current efforts to identify objective food biomarkers that will set the stage for transitioning to group discussion of topical concepts and challenges moderated by the speaker panel. Discussion topics will include food selection, experimental design, compound identification, and analytical and statistical approaches.

### Workshop Objectives

Provide knowledge about past and ongoing efforts to identify objective biomarkers of food intake, including the NIH/USDA Dietary Biomarker Discovery Consortium and other initiatives along with associated future opportunities for accessing samples and data, as well as perspectives on experimental approaches for food biomarker discovery and validation.

### Learning Outcomes

The workshop will be structured with a series of short introductory remarks on current strategies on how to identify objective food biomarkers with examples from FoodBall, the Periodic Table of Food Initiative, the Dietary Biomarkers Development Consortium and others. Speakers will set the stage to engage participants in active discussions on how to address challenges. The group discussion will be structured into several topics:

- Food types being tested and sample types that have or will be biobanked
- Study designs from cross-over to PK/PD-type studies
- Approaches for compound identification
- Validating tentative food biomarkers
- Potential uses of food biomarkers

The overall learning objective is to provide participants with the opportunity to learn about current approaches to food biomarker discovery and different perspectives on best practices.

*updated June 5*

METABOLOMICS SOCIETY

# W2: Public Data Re-use / Re-analysis with MetaboLights and GNPS

**Hands-On Session – Laptop Required

## Presenters

- **Thomas Payne** (EMBL-EBI)
- **Callum Martin** (EMBL-EBI)
- **Helena Mannochio-Russo** (UCSD)
- **Simone Zuffa** (UCSD)
- **Yasin El Abiead** (UCSD)
- **Pieter Dorrestein** (UCSD)

## Description

Metabolomics data deposition to public repositories such as MetaboLights and GNPS-MassIVE continues to grow. Latest statistics show over 163 and 557 TB data, 540,000 and 7,500,000 data files, respectively. Efforts to capture and standardize metadata, mandatory for MetaboLights and recommended for GNPS-MassIVE, empowers re-use / re-analysis of these data considerably. As part of this workshop, we share how to exploit metadata, with common vocabularies / ontologies, using annotations across 'organism', 'organism part', 'sample type', 'disease', etc, to derive new insights, create and test hypotheses, extend resources, or enable multi-omics. Simplifying data re-use / re-analysis for the community is of similar importance.

MetaboLights Labs (https://metabolights-labs.org) and GNPS2 (https://gnps2.org) will be showcased as two open-source, web-based examples working to achieve this. MetaboLights Labs provides tools and workflows for standardized NMR and MS analysis in Galaxy with homologous outputs to explore, test or integrate. GNPS2 provides an analysis hub for MS and MS/MS tools and workflows to access, visualize, search, annotate or identify spectra. This workshop will address a critical need to bring repositories and experts together to help the community get started in the re-use / re-analysis of public metabolomics data.

## Workshop Objectives

- Present the breadth and depth of metabolomics data available in the public domain
- Encourage community adoption and facilitate the re-use / re-analysis of public metabolomics data

## Learning Outcomes

- Access metabolomics data from public repositories
- Identify tools/workflows for public metabolomics data re-use / re-analysis
- Hands-on experience using public data with MetaboLights Labs and GNPS2

# W3: Untargeted Metabolomics, Molecular Networking, and Automatic Spectral Library Generation in MZmine

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

## Presenters


- **Tomáš Pluskal** (IOCB Prague)
- **Dr. Robin Schmid** (IOCB Prague)
- **Dr. Corinna Brungs** (IOCB Prague)
- **Dr. Tito Damiani** (IOCB Prague)
- **Dr. Louis-Felix Nothias** (Université Côte d'Azur)


## Description

Untargeted mass spectrometry (MS) experiments produce complex, multi-dimensional data that are practically impossible to investigate manually. Moreover, only a small fraction of the detected metabolites can be annotated, leaving a vast unknown chemical space to explore. This creates the need for flexible and scalable software solutions for MS data processing. MZmine is a modular platform-independent software with a vibrant open-source community. Recent contributions have expanded its capabilities to support various MS platforms, including chromatography-MS and MS imaging, combined with ion mobility spectrometry data. The interactive graphical user interface facilitates data exploration and results validation at each processing step. In addition, the MZmine Processing Wizard (MZwizard) introduces easy-to-configure workflows for metabolomics and lipidomics research that can be scaled to process large studies of thousands of samples.

This hands-on workshop will introduce the MZwizard, feature detection, compound annotation and molecular networking in MZmine, and existing bridges to GNPS and SIRIUS. We will also describe a novel mass spectral library generation workflow, including our efforts to expand open reference data. Using high-throughput analytical methods, we acquired multi-stage fragmentation spectra of 20,000 unique compounds in both polarities within 12 days in 4740 injections.

## Workshop Objectives

- Introducing untargeted metabolomics LC-MS/MS data processing in MZmine 3 with the MZwizard: Feature detection, compound annotation, and molecular networking
- Introducing MZmine tools for automatic generation of mass spectral libraries to advance open data sharing
- Exporting results from MZmine to interface other tools like SIRIUS and GNPS

## Learning Outcomes

- Getting an overview of MS data processing in MZmine by processing an example dataset
- Optimizing individual steps and understanding the distribution and shape of MS data
- Getting a clear workflow to acquire and generate open reference data

# W4: Demystifying Stable Isotope Labelling

**Hands-On Session – Laptop Optional

## Presenters

- **David de Souza**, Metabolomics Australia
- **Bart Ghesquiere**, VIB
- **James MacRae**, The Francis Crick Institute

## 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 in relating changes in identified metabolites to their roles in a given biological system. Understanding this relationship is critical for understanding the metabolic mechanisms in that biosystem.

Stable isotope labelling metabolomics 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. Such techniques can reveal subtle alterations in metabolic activity that would not be possible with unlabeled approaches. This extra depth of information can provide valuable insight into the mechanisms that underlie various physiological conditions and aberrant processes, including infection and disease.

However, this technique is perhaps not used as widely as it might. This workshop seeks to show how metabolic labelling studies are readily approachable and easily interpretable when performed correctly. We will show you how to design, run, and analyze stable isotope labelling experiments. We will explain how these simple workflows are often sufficient for significant biological insight.

This workshop is a mixture of traditional tutorials and some software demonstrations (laptops not essential, but would be useful).

## Workshop Objectives

- Know how to design a labelling project, including the essentials to consider and potential pitfalls
- Know the basics of analysis of labelling data, including a run-through 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

- Learn that stable isotope labelling projects are easy to design, perform, and interpret
- Labelling experiments can bring intricate detail to many metabolomics projects, whether untargeted or targeted, polar or lipid-focused
- Key principles behind data analysis workflows for labelling experiments, and how these differ when performed by LC-MS or GC-MS

# W5: SIRIUS 6 for Small Molecule Annotation using MS/MS Data

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

## Presenters


- **Dr. Kai Dührkop** (Friedrich Schiller University Jena)
- **Fleming Kretschmer** (Friedrich Schiller University Jena)


## Description

SIRIUS is a software suite that combines molecular formula annotation, structure database search and compound class annotation using MS/MS data (https://bio.informatik.uni-jena.de/sirius/). SIRIUS offers a user-friendly GUI and CLI that seamlessly integrates web-services for specific computational tasks. SIRIUS 6 provides methods for processing complete LC-MS/MS datasets, spectral library search, structure database search via CSI:FingerID, lipid annotation, de novo structure generation via MSNovelist, and combinatorial fragmentation for the verification of annotations. All compound annotations are provided in a unified view, to ease data analysis.

In this workshop, you will learn how to process whole LC-MS/MS datasets, annotate MS/MS with structural information, automatically obtain the most confident annotations from high-throughput experiments, and interpret the results in the GUI.

## Workshop Objectives

- Import/export data into and from SIRIUS
- Execute computational analysis (molecular formula, molecular structure and compound class annotations)
- Interpret SIRIUS results

## Learning Outcomes

You will be able to:

- Analyze whole datasets with multiple LC-MS/MS runs with SIRIUS
- Select suitable computational methods for your scientific question and perform a meaningful analysis
- Interpret and evaluate computed results and select confident annotations

# W6: Part 1 of 2

# Spectra Processing, Compound Annotation, Functional Insight and Causal Analysis using MetaboAnalyst 6.0

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

## Presenters

- **Jianguo Xia** (McGill University)

## Description

MetaboAnalyst (https://www.metaboanalyst.ca) is an easy-to-use, comprehensive web platform for metabolomics data analysis, interpretation and multi-omics integration. The tutorial aims to introduce participants to the key features of the most recent release of MetaboAnalyst (version 6.0) with focus on LC-MS spectra processing, compound annotation, advanced statistics, as well as causal analysis by leveraging mGWAS data.

During the workshop, participants will be given an overview of the main modules in MetaboAnalyst and most of their main functionalities. Selected example data sets will be processed by the instructor using different MetaboAnalyst features as part of a live demonstration. Workshop participants will continue with a "hands-on" lab session where they will be encouraged to use their own data and to process it following our 2022 Nature Protocols (doi: 0.1038/s41596-022-00710-w) together with new tutorials for more recent modules. Alternately, participants may work with "canned" data sets to explore MetaboAnalyst 6.0 on their own. The instructor (plus TAs) will assist participants in completing these tasks.

## Workshop Objectives

- To practice raw LC-MS spectra processing, MS2 peak annotation to functional insights
- To practice how to use MetaboAnalyst 6.0 to perform statistical analysis with complex metadata
- To practice how to link metabolomics data with genomics for causal analysis

## Learning Outcomes

- Become familiar with basic steps in LC-MS and MS/MS spectral processing and compound annotation
- To become familiar with functional analysis for metabolomics data
- To become familiar with common strategies for integration with other omics

***Part 2 of this workshop is immediately following at 4:30 p.m.**

## W6: Part 2 of 2

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### Learning Outcomes

- Become familiar with basic steps in LC-MS and MS/MS spectral processing and compound annotation
- To become familiar with functional analysis for metabolomics data
- To become familiar with common strategies for integration with other omics

***Part 1 of this workshop is immediately prior at 2:15 p.m.**

# W7: Reconnecting Lipidomics and Metabolomics for Metabolic Research

## Presenters

- **Matej Orešič**, *University of Turku, Finland:* Welcome and Introduction
- **Laura Goracci**, *University of Perugia, Italy:* Welcome and Introduction
- **Dajana Vuckovic**, *Concordia University, Montreal, Canada*: Harmonizing quality control strategies in metabolomics and lipidomics: path forward?
- **Michael Witting**, *Helmholtz Center Munich and TU Munich, Germany:* Shall I lean more towards the lipid or metabolite side of things?
- **Pieter Dorrestein**, *Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, UCSD, USA:* Kids and new kids on the block - molecular networking, lipid reference libraries and Query language tools to analyze metabolites and lipids

## Description

The variety and continuous interconversions of metabolites including lipids define the principles of life. Current research in metabolism aims to address the diversity and dynamics of small molecules in living cells in their full complexity. Historically, lipidomics has to a large degree grown into a separate field, often adopting different analytical methods, definitions and workflows. However, to understand metabolism at systemic scale, its close connectivity and regulations, one needs integrative solutions. This calls for bringing back together lipidomics and metabolomics fields.

This workshop is an initiative of the LipidMet Task Group of the Metabolomics Society and aims to bring together the expertise and experiences from both fields. The overall aim is to gather efforts in a synergistic way under the common umbrella of metabolic research with shared best practices, harmonization initiatives, and quality control procedures.

## Workshop Objectives

- To share practices and workflows closing the gap between metabolomics and lipidomics analytical solutions
- To discuss resources for data sharing
- To showcase the success of integrative metabolomics and lipidomics research, illustrating the power of combined knowledge and expertise

## Learning Outcomes

- Update on the sample preparation protocols, data acquisition, processing and analysis for metabolism research by combining the powers of lipidomics and metabolomics workflows, and presentation of resources for data sharing

# W8: Unveiling the mQACC Living Guidance for QA/QC Best Practices in LC-MS-Based Untargeted Metabolomics

## Presenters

- **Ping-Ching Hsu**, *University of Arkansas for Medical Sciences, USA:* Introduction to mQACC and the development of framework for best QA/QC practices
- **Callum Martin,** *EMBL-EBI, UK*: Living guidance document and website
- **Raquel Cumeras**, *Hospital Universitari Sant Joan de Reus, Institut d'Investigació Sanitària Pere Virgili, Spain:* Pooled QC samples – minimum & best practices
- **Dajana Vuckovic**, *Concordia University, Canada:* Internal standards – minimum & best practices
- **James Harynuk**, *University of Alberta, Canada*: Design of analytical batch – minimum & best practices

## Description

There is a critical need to standardize and implement QA and QC best practices in untargeted metabolomics to ensure high quality data generation and analysis. To address this need, the metabolomics Quality Assurance and quality Control Consortium (mQACC) was established in 2017 and currently has over 100 international members.

The goal of this workshop is to disseminate the key findings collected by mQACC Best Practices Working Group to the broader metabolomics community and launch an open-access best practices "living guidance" document and accompanying website, as a go-to resource for quality assurance and quality control (QA/QC) in untargeted LC-MS metabolomics. We will disseminate key practices identified through five years of community engagement across relevant technical areas: pooled/intra-study QC samples, use of internal standards, and analytical batch design.

Additionally, the workshop will act as a forum for critical discussions to further fine tune both format and content of the mQACC living guidance and encourage wide community adoption of best current practices.

## Workshop Objectives

- To disseminate findings from the mQACC Best Practices Working Group's extensive community engagement efforts to establish best practices for LC-MS data collection in untargeted metabolomics
- To solicit further feedback from the international metabolomics community on the open-access best practices living guidance document that will be freely accessible to researchers

## Learning Outcomes

- Attendees will learn about minimum and best practices for untargeted LC-MS-based metabolomics as proposed in living guidance by mQACC Best Practices Working Group. The guidance covered will include pooled QC, internal standards, and design of analytical batch
- Attendees will be able to identify how to participate in mQACC, including mechanisms to contribute to the best practices community engagement efforts and living guidance document

# W9: Planning your Career Development: Get Ahead by Getting Started!

## Presenters

- **Domenica Berardi**, Yale University
- **Thomas Vial**, Institut Pasteur
- **Aleš Kvasnička**, Palacký University Olomouc
- **Millena Barros Santos**, Bordeaux Metabolome-MetaboHUB
- **Silvia Radenkovic**, UMC Utrecht
- **Simone Zuffa**, University of California San Diego
- **Breanna Dixon**, University Of Manchester

## Description

This EMN workshop is for a diverse audience of ECRs from academic backgrounds, including Bachelor, Master students, PhD students, and postdocs, as well as ECRs in company/industry positions. We'll employ a step-by-step approach in identifying, improving and effectively communicating the skills necessary for future professional development. The workshop is divided into three sections:

- **"Step into your future career: planning and seeking skills":** providing a comprehensive background on effective strategies for skills identification and development
- **"How to effectively communicate your skills and experience on your CV and motivation letter: academia and industry perspectives"**: provide practical directions for writing impactful CV/motivation letters and imparting self-promotion strategies vital in the competitive job market
- Open discussion between the ECR audience, EMN members and invited panelists from academia and industry. This will provide the opportunity to discuss with panelists personal challenges in skills development and improvement, and to learn – based on their experiences – strategies to adapt and/or overcome these challenges

## Workshop Objectives

- Identify the professional and personal skill sets which are necessary for the next career move, therefore addressing skill gaps and opportunities to overcome/improve them to respond effectively to career challenges
- Learn strategies of self-promotion in the process of networking and present yourself as a skilled professional in your field of expertise, therefore promoting your growing career in the future. Learn how to prepare an effective CV, motivation letter and marketing strategies to make CV/motivation letter work for the next career move in science with a focus on metabolomics research
- Share experiences and learn from the career path of professionals working in academia and/or industry. Acknowledge and reflect on the challenges faced by underrepresented groups in academia and industry, which represent barriers towards professional development

## Learning Outcomes

- Skill Identification and Gap Analysis: ECRs will learn methods to identify and evaluate their existing skill sets, both technical and soft skills, necessary for their career goals in academia or industry. Ascertain the importance of adaptability qualities needed to navigate diverse career landscapes, providing guidance on developing skills like cross-cultural communication, resilience, and problem-solving to address career challenges effectively
- Career Path Exploration: gain insights into the skills essential for various career paths within academia and industry, aiding in informed decision-making about their professional trajectory
- Skill Enhancement Strategies and Promotion: learn different strategies and resources available to enhance and develop identified skills, and how to communicate them when applying for a job or being interviewed including practical exercises, workshops, online courses, mentoring, or other professional development avenues.
- CV and Motivation Letter: Guidance on effectively translating identified skills into impactful CV/resume content and motivation letter, strategically communicating these skills to potential industrial employers or academic institutions
- Self-Reflection and Goal Setting: Encouraging ECRs to reflect on their career aspirations, enabling them to set clear, achievable goals and develop action plans to reach them, tips on building cross-cultural competencies, networking internationally, and leveraging diverse experiences

# W10: Improving Data Analysis for Ambient Ionisation and Direct Infusion MS-based Metabolomics

## Presenters

- **Dr. Nicholas Birse** (Queen's University Belfast, UK)
- **Dr. Vera Plekhova** (Ghent University, Belgium)
- **Ir. Nicolas Defooz** (Ghent University, Belgium)
- **Prof. Lynn Vanhaecke** (Ghent University, Belgium)

## Description

The speed and simplicity of ambient ionization and direct infusion mass spectrometry (AIMS-DIMS) platforms have made them increasingly popular methods for rapid sample screening. However, data handling techniques have become inconsistent as vendor-specific tools are replaced by custom processing pipelines that best fit specific workflows. While tailored approaches aim to leverage the speed and versatility of AIMS-DIMS, they complicate data reproducibility and validation, which is already challenging throughout various instrumental configurations.

The workshop will host an expert panel, well-versed in both vendor and non-vendor data processing tools and pathways. They will discuss the features and utility of their toolset, as well as strategies for improving the reproducibility of their workflows. The level will be appropriate for a broad range of expertise, from graduate students to experienced investigators. To target emerging topics of interest the workshop will include lightning talks from speakers and posters presenters participating in the conference and representatives from both academia and instrument and software vendors.

There will be a Question-and-Answer session with the panel. The workshop will conclude with a set of practical outcomes and recommendations to mass spectrometry users, instrument and software developers, on how to advance the application of AIMS-DIMS within the metabolomics area.

## Workshop Objectives

- Quality control for AIMS-DIMS-based metabolomics: developing strategies to ensure data acquisition is robust and comparable across instruments and platforms
- Data processing: investigating ways to ensure data processing is directly comparable when using different software packages and programs, including strategies relying on direct extraction from raw files (no peak picking)
- Reproducibility: assessing strategies for making data reproducible both within the same laboratory and across multiple laboratories considering the prior 2 objectives and other considerations necessary for AIMS-DIMS-based metabolomics platforms

## Learning Outcomes

- System setup and acquisition: participants are expected to understand existing and emerging strategies for evaluating and ensuring appropriate setup, calibration and stability of AIMS-DIMS platforms throughout the analysis as a quality assurance measure for the acquired metabolomic data
- Data analysis: participants are expected to understand ways of processing AIMS-DIMS data with different software packages, aiming for consistent results and outcomes. Similarly they should develop a greater understanding of where software output may diverge and the challenges related to maintaining reproducibility
- Reproducibility: participants are anticipated to comprehend the concept of reproducibility and how to obtain high levels of reproducibility during both AIMS-DIMS metabolomics data acquisition and processing and how to maintain reproducible results across different laboratories and data sets where relevant

# W11: Metabolomics Infrastructure and Facility Forum: Sharing Good Practices and Avoiding Pitfalls

## Presenters

- **Fabien Jourdan**, Director of MetaboHUB
- **Floriant Bellvert**, Assistant Director of MetaboHUB
- **Anne-Emmanuelle Hay**, Project Manager of MetaboHUB
- **Pierre Petriacq**, Leader of Node MetaboHUB-Bordeaux
- **David Wishart**, Director of TMIC (The Metabolomics Innovation Centre, Canada)
- **Coral Barbas**, Director of CEMBIO (The Centre of Metabolomics and Bioanalysis, Spain)
- **Francisco Javier Rupérez,** CEMBIO, Spain
- **Monica Cala**, Metcore Director, Colombia

## Description

Metabolomics is a research area with a large range of applications in plant, biotechnologies, environment and human health. Due to its strong technological and multidisciplinary requirements, data production is often provided by platforms ranging from lab scale to national infrastructures.

Setting up facilities and infrastructures is a rewarding journey with plenty of opportunities but also challenges. Through this workshop, we will open a forum where experiences could be shared and where early-stage facility managers and staff could find fruitful information to avoid pitfalls and provide high-level metabolomics services to the scientific community.

Beyond management, this workshop will also be the opportunity to share experiences by Early Career Researchers (ECR) on the benefit of R&D in the framework of platforms and discuss how to promote ECRs.

The following challenges will be discussed:

- Service access, dealing with requests
- Multisite infrastructures (interoperability)
- Training (initial and continuous)
- Technology transfer and spin off creations
- Data management and open science
- How to attract (and keep) talented ECR
- Balance between R&D and service

We will also open two round tables on:

- Interactions between non-academic and academic sectors
- Creation of MetSoc facility and infrastructure task group

## Workshop Objectives

- Learn from the success of other infrastructures, hence creating emulation and advanced metabolomics services for the future
- Aim to create an international network of facilities and infrastructures so we can increase the quality and openness of metabolomics services
- Consider how we can articulate between academic and non-academic service providers for a two-way benefit

## Learning Outcomes

- Early-stage facility managers and staff will have the opportunity to learn from more advanced platforms, hence gaining time and efficiency for their settlements
- ECR will discover that working within facilities can provide exciting methodological and technical challenges to tackle
- Metabolomics facility will gain knowledge to move further in terms of FAIR data production, EDI consideration, technology transfer and ECR promotion. This FORUM will potentially spearhead a new task group within the Society.

# W12: FAIR and Open Data Sharing through Public Repositories

## Presenters

- **Masanori Arita,** National Institute of Genetics / RIKEN Center for Sustainable Resource Science, Japan

## Description

In this workshop we will introduce major public repositories for metabolomics and proteomics data, and the status of coordination and standardization. Data submission/curation is not an easy task; we need to design proper incentives for data submitters as well as data curators to achieve accumulation of data with better quality and availability. Also important is the coordination and collaboration among data platforms so that researchers as well as our funders can recognize and support our activities.

In this workshop, we encourage interaction/discussion among participants so that we can improve our services through international collaboration.

## Workshop Objectives

How to make your data reusable in a sustainable way

## Learning Outcomes

Better communication among data submitters, users, and repositories

# W13: MALDI-MS Imaging Tool for Medical Prognosis/Diagnosis: Applications and Perspectives

## Presenters

- **Dr. Boutayna Rhourri**, Montreal University/Bordeaux University, Canada

## Description

In the last 2 decades, mass spectrometry imaging (MSI) has gained significant traction in the field of disease diagnosis and prognosis due to its ability to provide detailed spatial and molecular information about biological samples. Advances in mass spectrometry instrumentation have led to improved spatial resolution that allows for the precise localization of molecules within tissues, aiding in the identification of specific regions associated with disease pathology.

Integration with other omics technologies, such as genomics, transcriptomics, and proteomics, MSI allows for a more holistic understanding of the molecular changes associated with diseases and facilitates the discovery of novel biomarkers associated with diseases.

In this workshop, we'll go through mass spectrometry imaging processing from sample preparation to data analysis.

## Workshop Objectives

Initiate attendees to MSI workflow:

- Sample preparation
- Matrix application
- Instrumentation
- Data analysis

## Learning Outcomes

- Learn how to prepare sample for MSI
- Learn the type of matrices for MALDI-MS-Imaging and methods of application
- Learn how to optimize the instrument for MSI acquisition
- Learn different preprocessing and post processing step for MSI data analysis