

Pre-Conference Workshops

Sunday, June 18

12:00 p.m. – 2:00 p.m.

W1: Ion Mobility-Mass Spectrometry Workflows for Metabolomics

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

Presenter

- **Kelly Hines**, University of Georgia: Introduction to IM-MS Workflows
- **Markace Rainey**, Georgia Institute of Technology: CCS Prediction Methods
- **Christine Chang** and **Jess Bade**, Pacific Northwest National Laboratory: DEIMoS
- **Tomáš Pluskal**, Institute of Organic Chemistry & Biochemistry, Czech Academy of Sciences: MZmine 3

Description

Ion mobility-mass spectrometry is a rapid, gas-phase method that provides information on the size and mass of ions. The structural information encoded in the IM dimension, known as a collision cross section (CCS), can be valuable evidence for the assignment of identifications to unknown metabolite features. Modern IM-MS instruments are capable of resolving powers that are sufficient to resolve isomeric metabolites within complex mixtures. Datasets generated by IM-MS are incredibly rich with information, especially when coupled to chromatographic separations and incorporating data-independent acquisition of tandem MS spectra. The novelty and complexity of IM-MS data presents unique challenges for the performance of traditional untargeted metabolomics workflows. Compared to the wealth of options for LC-MS/MS data processing, software capable of extracting information from the IM dimension of multi-dimensional IM-MS, IM-MS/MS, and LC-IM-MS(/MS) datasets are limited. This workshop will introduce attendees to the metabolomics software packages that utilize the IM dimension in peak picking, alignment, and feature identification. Workflows based on freely available and open-source options will be demonstrated during the workshop. Finally, resources for metabolite annotation using CCS databases and CCS predictions will be highlighted.

Workshop Objectives

- Introduction to available software options for processing and analyzing IM-MS data;
- Demonstration of data analysis and interpretation workflows for IM-MS data;
- Emphasis on freely available, open-source options;
- Tutorial on prediction of IM collision cross sections by machine learning using freely available software.

Learning Outcomes

- Identify software that is suitable for processing IM-MS data from various sources;
- Navigate file conversion into vendor-neutral formats using real life data files;
- Process IM-MS data in both targeted and untargeted methods;
- Utilize CCS databases and prediction tools to facilitate identifications

W2: The Future Potential of Metabolomics for Illuminating the Molecular Dark Matter of Soil

Presenters

- **Kirsten Hofmockel**, Pacific Northwest National Laboratory
- **Joëlle Sasse Schläpfer**, Universität Zürich
- **Myrna Simpson**, University of Toronto Scarborough
- **Sean Brady**, The Rockefeller University
- **Adam Hollerbach**, Pacific Northwest National Laboratory

Description

The exchange of carbon between plants and soil initiates important plant-microbe interactions that form soil organic matter and release greenhouse gases. Plant metabolites select for specific microbial communities and pathways that define the chemistry of dissolved organic matter in soil. The chemistry of these extracellular metabolites influences the potential for carbon to be sequestered onto charged surfaces of soil minerals. This rich mixture of small molecules is not well-annotated or understood. Compounding this, the physical make-up and properties of soil can prevent the full extraction of molecular constituents due to strong interactions with particulate and mineral surfaces, limiting our perspective of the molecular landscape present or potential pathways to enhance soil carbon sequestration.

Finally, analytical methodologies that are most efficient in the confident identification of metabolites rely on data from analyses of authentic chemical standards. This is a particularly significant limitation in studies of molecules in soil where chemical standards are not available for the majority of molecules. New analytical approaches are needed for comprehensively and accurately determining the chemical identities of the molecules therein. In this workshop we will explore challenges and opportunities for exploring small molecule identification within the dark matter of the soil metabolome.

Workshop Objectives

- Introducing the metabolomics community to challenges of comprehensively and accurately measuring the soil metabolome,
- Discussion of strategies and new technologies for greatly improved elucidation of molecular speciation in soil.

Learning Outcomes

- Learn the relevance of plant-microbe communities and soil metabolomes for climate change,
- Learn the knowledge gaps and analytical challenges associated with measuring the soil metabolome.

W3: Meta-analysis, biomarker discovery, and pathway enrichment analysis of metabolomics data

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

Presenters

- **Ali Rahnavard**, George Washington University
- **Chiraag Gohel**, George Washington University

Description

Methodological advancements paired with measured multi-omics data using high-throughput technologies enable capturing a comprehensive snapshot of distinct biological entities. In particular, low-cost, culture-independent omics profiling has made metabolomics surveys of human health, other hosts, and the environment feasible at an unprecedented scale. The resulting data have stimulated the development of new statistical and computational approaches to analyze and integrate omics data, including human gene expression, microbial gene products, metabolites, and proteins, among others.

Metabolomics data generated from diverse platforms are often analyzed individually; we aim to combine metabolite profiles and feed them into generic downstream analysis software with proper appreciation of the data's statistical properties, resulting in more powerful results and biological inferences. Further, there is also an overwhelmingly extensive collection of downstream analysis software platforms, and appropriately selecting the best tool can be difficult for untrained researchers and non-specialists.

Also, we present a high-level introduction to computational multi-omics, highlighting the state-of-the-art in the field and outstanding challenges geared towards downstream analysis methods. The workshop will include formulating biological hypotheses and identifying the statistical methods currently available to achieve them. The workshop is project-focused and uses a hands-on approach. Participants are encouraged to attend with a specific study or project in mind for the application of the workshop content in the short term. The workshop will use real data for the exercises.

Workshop Objectives

- Attendees will use tools for metabolomics meta-analysis through multi-study data scaling, integration, and harmonization using *massSight* tool.
- Attendees will use tools for pattern discovery in multi-omics with metabolomics data, including:
 - *omeClust*: Omics community detection using multi-resolution clustering,
 - *Tweedieverse*: A unified statistical framework for differential analysis of multi-omics,
 - *omePath*: omics pathway enrichment analysis interspersed with lecture content, attendees will work through multi-omics analysis tutorials.
- Attendees will practice generating publication-quality figures and effective visualization of the results.

Learning Outcomes

- Be able to apply novel techniques (such as *massSight*) to combine metabolite profiles and perform meta-analysis of metabolomics data.
- Understand statistical properties of metabolomics data and challenges for multivariable association testing in population-scale meta-omics studies.
- Understand how to apply pathway enrichment analysis to metabolomic data using a variety of statistical methods implemented in *omePath*.
- Be able to perform a meta-analysis of metabolomics datasets by combining multiple studies data and perform pairwise association testing with other omics profiles in population-scale datasets.

W4: Emergent Technologies in NMR Metabolomics

Presenters

- **Art Edison**, University of Georgia: ¹³C-probes and high-field GHz NMR
- **Goncalo Gouveia**, University of Maryland and National Institute of Standards and Technology: LC-MS-SPE-NMR methods
- **David Wishart**, University of Alberta: NMR spectral prediction
- **Elizabeth O'Day**, Olaris Therapeutics: Clinical applications of NMR metabolomics
- **Bob Powers**, University of Nebraska-Lincoln: Improve the coverage and quality of NMR met data

Description

As one of the major metabolomics investigation methodologies, NMR has its unique advantages, including simplicity in sample preparations, an ability to investigate physical and chemical properties, and in vivo evaluations through metabolomics imaging and In-cell NMR. Comparable to other scientific endeavors, advancements and methodology developments of NMR-metabolomics continues to progress at a rapid pace, making it challenging for new investigators to keep pace with emergent technologies. The workshop aims to collectively and concisely summarize multiple frontiers of NMR-metabolomics advancements, and to inspire attendants to adopt/implement the new developments and applications of NMR-metabolomics into their own research.

This workshop will review and examine current technological advancements in NMR-metabolomics, and highlight recent achievements in various research fronts while acknowledging aspects that require further research attention. Expert discussions will cover: the application of cutting-edge ultra-high field (GHz) NMR for different scientific disciplines and technological advancements in probe design, integration of NMR- and mass spectrometry (MS)-metabolomics to improve the reliability, accuracy, and coverage of data, the application of artificial intelligence and deep learning to NMR spectral predictions to annotate the vast number of unknown metabolites, technological transfer of NMR-metabolomics to the clinic, and new methods to improve the coverage and quality of NMR-metabolomics data.

Workshop Objectives

- Disseminate to the metabolomics community recent technological advancements in the application of NMR to metabolomics to adopt into their research programs
- Understanding the current state of the art in NMR-based metabolomics and its value to different scientific disciplines to facilitate the routine combination of NMR and mass spectrometry for metabolomics studies
- A novice will learn how different NMR methodologies are applicable to a variety of metabolomics studies
- Understand current issues and limitations to improve the coverage and quality of NMR metabolomics data

Learning Outcomes

- For attendees working in areas of NMR metabolomics or metabolomics in general, the workshop will provide an opportunity to consider various areas of the field and be informed with new NMR approaches.
- For non-NMR attendees, in addition to learn information on the landscape of the current NMR metabolomics fields, they may appreciate the enhance metabolomics power when MS is assisted by NMR.

NEW! W5: Hands-on analysis of mass spectrometry-based metabolomics and exposomics big data using ADAP****Hands-On Session – Laptop Required****Presenters**

- **Xiuxia Du**, University of North Carolina at Charlotte

Description

This workshop will first introduce the ADAP informatics suite of software tools and cloud resources designed specifically for handling untargeted mass spectrometry-based metabolomics and exposomics big data from large-scale studies. With a working knowledge of ADAP, the workshop participants will learn to use these ADAP informatics tools through hands-on exercises. Specifically, participants will learn how to use the: (1) desktop software tool ADAP-BIG for extracting compound-relevant signals from raw LC-MS and GC-MS data, and (2) cloud resource ADAP-KDB for identifying and annotating the resulting signals by matching against in-house and publicly available compound databases.

Workshop Objectives

- To educate researchers on how to use ADAP-BIG and ADAP-KDB
- To solicitate feedback from participants about how to improve ADAP-BIG and ADAP-KDB to meet the community's needs

Learning Outcomes

- To understand the principle of ADAP-BIG in extracting signals from complex LC-MS and GC-MS raw data
- To be able to use ADAP-BIG and ADAP-KDB for preprocessing raw LC-MS and GC-MS data and identifying and annotating resulting signals using ADAP-KDB
- To understand how to determine appropriate analysis parameters

W6: Multi-Platform Metabolomics Workflows: The role of modern day, high performance GC-MS as a vital, enhancing, and complimentary tool

Presenters

- **Catherine Winder**, University of Liverpool, UK - Introduction to Successful Experimental Design and QA/QC principles for Metabolomics
- **Luis Valdiviez**, University of California (Davis), USA - Introduction to GC-TOFMS and its importance in non-target and semi-target metabolomics workflows
- **Brian Ruddy**, Corteva Agriscience, USA - Critical Components of a Large-Scale GC-TOFMS Approach to Green (Plant) Metabolomics Workflows
- **Pierre-Hugues Stefanuto**, University of Liege, Belgium - Comprehensive two-dimensional GC (GCxGC) examples for enriching numbers of species detected and annotated, in non-target and semi-target analyses where matrix complexity is high, and identification confidence can be aided
- **David Alonso**, LECO Corporation, USA - Utilizing GCxGC with high resolution MS for discovery workflows – Strategies for unknown identification and overall increased confidence in compound annotation will be discussed, highlighting a multi-mode ionization source and important software tools
- **Heather Bean**, Arizona State University, USA - Addressing data analysis challenges involving large complex sample set studies

Description

The vast collection of metabolites present in biological systems, i.e. the metabolome, is chemically diverse. In discovery-based, untargeted metabolomics where the goal is to detect and annotate as many metabolites as possible, the use of complementary analytical platforms is extremely important. No single analytical platform is capable of characterizing the degree of chemical diversity present in these types of samples on its own. That is why it is important to employ multiple analytical techniques, such as GC-MS, LC-MS, and NMR to gain the greatest amount of information. This workshop will focus on the importance of GC-MS workflows and their role in the non-targeted and semi-targeted investigation of primary and secondary metabolites in biological systems.

The segments of the metabolomics workflow which will be covered in this workshop include:

- 1) effective experimental design creation,
- 2) the importance GC-TOFMS's role in non-targeted metabolomics,
- 3) critical components of large-scale metabolomics studies,
- 4) advanced chromatographic separation techniques to improve metabolite detection and annotation when matrix complexity is high,
- 5) the use of high-resolution MS strategies for discovery workflows where identification of unknown metabolites is of utmost importance, and lastly,
- 6) strategies for data analysis of large complex sample sets.

Workshop Objectives

- Highlight the key advantages of high-performance GC-MS for routine metabolomics research.
- Increase awareness of the critical role modern GC-MS instrumentation plays in complementary multi-platform metabolomics.
- Address the fundamental requirements of each step of metabolomics workflows, including QA/QC protocol design, technology/instrumental choice for confidently solving challenges in different assays, and automated data processing and visualization.

Learning Outcomes

Attendees will gain a broader understanding of the key attributes to consider in successfully employing GC-MS metabolomics workflows. Everything from experimental design and QA/QC, to sample preparation (automated Derivatization), to routine and advanced sample analysis techniques, and finally data processing and statistical analysis strategies, will be covered.

W7: EMN Workshop – Professional Career Development: Steps Towards Independent Research

Presenters

- Section 1 - Create your research niche (Academic/PI)
- Section 2 - Developing your portfolio beyond benchwork (Academic PI)
- Section 3 - Learn about funding applications (Funder/Research Council)
- Section 4 - Learn about the different requirements of lectureship applications (Career Coach)

Description

This EMN workshop is targeted towards ECRs including Masters students, PhD students, and postdocs. The workshop is divided into four parts:

- 1) Creating your research niche;
- 2) Developing your portfolio beyond your research e.g. teaching and service;
- 3) Starting to think about your funding applications;
- 4) Lectureship (tenure/tenure track) - 'Where to start'.

The workshop will include speakers from a variety of sectors and expertise such as academia, funding agencies, and career advisors. It will also include an interactive open discussion session with time for ECR to discuss with the speakers the challenges they faced, what they learnt and how they adapted from these situations while developing their own research program.

Workshop Objectives

- Identify how you can develop your own research area and scientific niche
- Learn about tools and resources that will allow ECR to improve their transferable skills, including teaching, mentoring, networking, collaborating, managing, to developed portfolio beyond their research interest.
- Learn about the process of putting a fellowship application together, or how to join as co-investigator or trainee on grants.
- Learn about different aspects that are required for the next step (tenure positions) in your career towards independence.

Learning Outcomes

- ECRs will familiarize with their research interest while developing a leading niche in the scientific community.
- Get insights of the tools available to improve their leadership, management and communication skills towards building a strong scientific profile inside and outside the lab. This will include how to present yourself and your scientific work to the community, and how to manage multiple responsibilities and tasks as an independent researcher. (e.g. teaching, publishing, mentoring, etc).
- Identifying appropriate funding, important aspects of writing a postdoctoral fellowship.
- Learn about the different requirements of lectureship applications, i.e. what to write in your cover letter, resume, teaching and research statements.

W8: Part 1 of 2

Using MetaboAnalyst 5.0 for high-throughput LC-MS and tandem MS spectral processing, annotation, and multi-omics integration

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

Presenters

- **Jeff Xia**, McGill University

Description

Liquid-chromatography coupled with tandem mass spectrometry (LC-MS/MS) has become the most popular approach for various global metabolomics studies across biomedical and environmental sciences. This workshop aims to introduce three new features of MetaboAnalyst (www.metaboanalyst.ca). We will start with our integrated LC-MS and MS/MS spectra processing pipeline that enables high-throughput, sensitive peak detection, MS/MS data deconvolution (for both data dependent and SWATH-independent acquisition), and comprehensive database-assisted annotation. The resulting annotated table will be used to illustrate our unbiased functional enrichment analysis module, which accepts compounds, LC-MS peaks or mixed input types via unified interface. Finally, we will showcase how to integrate metabolomics data with SNPs and microbiome data to understand host-microbiome interactions.

The three new features have long been requested by the MetaboAnalyst user community. We have made significant efforts to develop highly efficient functions with few tuning parameters that are suitable for web-based platform as well as the MetaboAnalystR package for local installation. These features facilitate harmonized metabolomics data analysis, interpretation and systems biology. A detailed step-by-step vignette will be made available for workshop attendees to follow during and after the workshop.

Workshop Objectives

- Understand the key steps involved in LC-MS and tandem MS spectra processing and peak annotation
- Be aware of potential bias in current pathway analysis; to learn some common strategies in multi-omics integration

Learning Outcomes

Using MetaboAnalyst 5.0 for streamlined LC-MS1 and MS2 processing, annotation, pathway analysis and integration with common omics data.

***Part 2 of this workshop is immediately following at 10:30 a.m.**

W9: Moving Toward Consensus: mQACC Community Engagement on Best QA/QC Practices in LC-MS-Based Untargeted Metabolomics

Presenters

- **Jonathan Mosley**, U.S. Environmental Protection Agency, USA: Introduction to mQACC and QA/QC principles
- **Rick Dunn**, University of Liverpool, UK: Quality of metabolite identification/annotation
- **Tracey Schock**, National Institute of Standards and Technology, USA: Use of Reference Materials
- **Dajana Vuckovic**, Concordia University, Canada: Data Quality Review
- **Matthew Lewis**, Bruker Life Sciences Mass Spectrometry, UK: Quality Assurance
- **Jonathan Mosley**, U.S. Environmental Protection Agency, USA: Open Discussion on Living Guidance Document

Description

High quality data generation and analysis is critical for the success of untargeted metabolomics and can be achieved through standardization and implementation of best QA and QC practices. In an effort to define and promote QA and QC practices, the metabolomics Quality Assurance and quality Control Consortium (mQACC) was established in 2017 and currently has over 90 international members. The mQACC Best Practices Working Group has actively engaged the metabolomics community over the last four years through a combination of eleven (virtual and in-person) interactive forums and workshops with a total attendance exceeding 600 participants across all events. In 2022, the working group hosted a workshop to disseminate findings from four key QC areas to the broader metabolomics community. The enthusiastic and critical discussions contributed towards building an open-access best practices “living guidance” document that reflects the community feedback received.

This year’s workshop will build on the successful 2022 event with four additional focus topics: quality of metabolite identification/annotation, use of reference materials, data quality review, and quality assurance practices for LC-MS based untargeted metabolomics research. Please join us and add your experience to the QA/QC guidance document that will become the go-to resource for metabolomics scientists.

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 compiled and summarized findings to establish an open-access best practices “living guidance” document that will be freely accessible to researchers.

Learning Outcomes

- Attendees will understand the community feedback received by the mQACC Best Practices Working Group and recognize how the feedback will be used to support QA/QC best practices for untargeted LC-MS-based metabolomics.
- Attendees will be able to identify how to participate in mQACC, including mechanisms to contribute to the best practices community engagement efforts.

W10: Data preprocessing in non-targeted metabolomics – best practices and pitfalls

Presenters

- **Kati Hanhineva**, University of Turku, Finland
- **Ville Koistinen**, University of Turku, Finland
- **Topi Meuronen**, University of Turku, Finland
- **Retu Haikonen**, Institute of Public Health and Clinical Nutrition, University of Eastern Finland, Finland

Description

Non-targeted metabolite profiling assays involve various specialized data-analytical steps between the acquisition of the raw data files all the way to the final compound lists reported in publications. Whilst the peak collection, statistical analysis, and compound identification procedures have gained much attention, another important step in the data-analysis workflow is the data pre-processing prior entering to the statistical analysis and compound annotation. These steps include e.g. quality control metrics, data imputation, drift correction, scaling/normalizing/transformation, combination of features originating from the same compound etc. These procedures affect the workflow in general and will have an impact on the quality of data entering the feature selection procedure and thus will impact the final outcome of the analysis. During the workshop, an overview and best practices will be presented and discussed. As one example is the pipeline “notame” developed in our group.

Workshop Objectives

Workshop participants have the possibility to familiarize with the different available online tools for the non-targeted metabolomics data preprocessing. The participants will have introduction on the available resources online and possibility for hands-on training with some of the selected approaches will be investigated.

Learning Outcomes

Workshop participants will understand the necessity for various data preprocessing steps between the creation of the first raw data matrix after data collection/peak picking and the eventual dataset entering the statistical assessment and compound identification. The participants will have introduction on the available resources online.

W8: Part 2 of 2**Using MetaboAnalyst 5.0 for high-throughput LC-MS and tandem MS spectral processing, annotation, and multi-omics integration******Hands-On Session – Laptop Required****Presenters**

- **Jeff Xia**, McGill University

Description

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The three new features have long been requested by the MetaboAnalyst user community. We have made significant efforts to develop highly efficient functions with few tuning parameters that are suitable for web-based platform as well as the MetaboAnalystR package for local installation. These features facilitate harmonized metabolomics data analysis, interpretation and systems biology. A detailed step-by-step vignette will be made available for workshop attendees to follow during and after the workshop.

Workshop Objectives

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Learning Outcomes

Using MetaboAnalyst 5.0 for streamlined LC-MS1 and MS2 processing, annotation, pathway analysis and integration with common omics data.

W11: Interdisciplinary Metabolomic Epidemiology: The Pathway to Clinical Translation

Presenters

- **Krista Zanetti**, Ph.D., M.P.H., R.D.N, NIH Office of Nutrition Research
- **Craig Wheelock**, Ph.D.; Karolinska Institute (Biochemist)
- **Lining Guo**, Ph.D.; Precion Inc. (Biochemist)
- **Deeba Husain**, M.D. Massachusetts Eye and Ear; Harvard Medical School (Clinician)
- **Jessica Lasky-Su**, Sc.D.; Brigham and Women's Hospital and Harvard Medical School (Epidemiologist)

Description

The power of large metabolomic epidemiology studies has enabled the identification of multiple robust associations between metabolites and disease with the potential to provide critical insight into disease processes and clinical translation. However, promising findings often fall short due to lack of the necessary domain expertise to assure follow-up steps are comprehensive enough to translate findings to the clinic. Crosstalk between domain experts is imperative, but the practical implementation of interdisciplinary research teams is often not fully recognized. Starting with the identification of a metabolite-disease association, this workshop will identify the roles that other critical domain experts -- biochemists, clinicians, statisticians, data scientists, etc. -- play to further enable biological understanding and clinical translation from epidemiological studies.

Four domain experts will provide their perspective and discuss the importance of their distinct roles in interdisciplinary collaborations that include:

- 1) assuring accurate biological interpretation;
- 2) identifying key metabolites that are best suited to follow-up as clinical biomarkers;
- 3) formulating clinically relevant questions to inform next steps of research; and
- 4) ensuring analytic robustness of findings.

The workshop will include dynamic discussions between the domain experts and workshop attendees that will examine key approaches for successful interdisciplinary collaborations to enable clinical translation.

Workshop Objectives

- Describe the important roles that distinct domain experts play in the process from discovery to clinical translation in metabolomic epidemiology.
- Identify important areas where crosstalk between domain experts is currently lacking.
- Identify specific steps that can be taken to better establish a multidisciplinary team for metabolomic epidemiology research that will promote moving initial discovery to clinical translation.

Learning Outcomes

- Attendees will understand a general framework that can be used for effective multidisciplinary collaborations in human health research.
- Attendees will walk away with concrete strategies to build multidisciplinary collaborations.
- Attendees will gain an appreciation that working collaboratively is the most effective way to identify research strategies that lead to clinical translation.

W12: Data Standardization and Reuse through Public Repositories

Presenters

- **Claire O'Donovan**, EMBL-EBI - MetaboLights
- **Masanori Arita**, NIG - MetaboBank
- **Shankar Subramaniam**, USC – Metabolomics Workbench

Description

The importance of data reuse cannot be over-emphasized since the beginning of the digital age. A recent game changer in the field of metabolomics is that the major journals and funders now mandate data submission to publicly traceable repositories which has led to an exponential growth in public data. This has highlighted the need for repositories and the wider community to reinvigorate standards and collaborations. In this workshop we, the providers of the major public metabolomics repositories, will present the current state of the art guidelines for experimental design including protocols, metadata, and result description. A data management plan (DMP) should be an integral part of any experimental design and we will present strategies towards metabolomics data management. After introducing our public repositories and their function in the research community, we will also discuss the ways to create synergy among researchers and other resources through data reuse and standardization.

Workshop Objectives

- To present the current state of the art of metabolomics study submission and curation
- To gather feedback and requirements from our user communities
- To enable the repositories to establish a collaborative plan for the future

Learning Outcomes

- To understand the current state of the art of metabolomics study submission
- To engage with repository staff and contribute to the future development of those resources for their benefit