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Metabolomics Society News

Members Corner

Early-Career Members Network (EMN)



New Committee Members

The EMN has appointed and is very happy to introduce its new committee members for the year 2019-2020. Read their bios and meet them [here](#). We are proud to have representatives from across the world and from diverse backgrounds. Stay tuned for all the exciting projects we are working on.

Travel Bursary Program

The call for applications for the EMN Travel Bursary Program will be announced early in January on the Metabolomics Society website and mailing list and on our social media. Up to four travel grants will be awarded to early-career researchers to cover travel, accommodation costs and conference fees up to \$500.

EMN Social Media

Follow the EMN on [Facebook](#) and [Twitter](#) for updates and special events.

The Metabolomics Society is an independent non-profit organisation dedicated to promoting the growth, use and understanding of metabolomics in the life sciences.

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Membership Enquiries

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MetaboNews is a monthly newsletter published in partnership between The Metabolomics Innovation Centre (TMIC) and Metabolomics Society.

An advertisement for ChenomX NMR Mixture Analysis. The top part features the "CHENOMX" logo with "NMR Mixture Analysis" underneath. Below this, the text "Isolate and Identify hundreds of compounds using the Profiler Module" is displayed. The bottom half of the ad shows a close-up of several test tubes in a rack, with a green hexagonal molecular structure overlaid on them. At the very bottom, the website "www.chenomx.com" is listed on an orange background.

CHENOMX
NMR Mixture Analysis

Isolate and Identify
hundreds of
compounds using the
Profiler Module

www.chenomx.com

SpOtlight

Open, Transparent and Reproducible Data Science in Clinical Metabolomics using Jupyter Notebooks and Cloud Computing.

Feature article contributed by:

David Broadhurst, Centre for Integrative Metabolomics & Computational Biology
[Edith Cowan University, Perth, Western Australia](#)

Most of us are familiar with the generic lifecycle of a clinical metabolomics study. We first propose a hypothesis, then design a study, obtain samples, choose an assay, design an analytical experiment, acquire raw data, deconvolve into a data matrix, annotate metabolite peaks, perform quality control (data cleaning), extract predictive/statistical insights from data, interpret biochemically, disseminate findings, and finally generate further hypotheses or translate knowledge into practice. As **Figure 1** suggests, we often loop through subsets of these stages multiple times.

In terms of data management, each stage in the lifecycle is a discrete process (or workflow) to which data integrity checks can be applied to ensure validity and accuracy. After which data can be locked down (archived) before proceeding to the next stage. Parts of the lifecycle can be semi-automated using off-the-shelf standard operating procedures. Typically a metabolomics lab will have a small number of generic (biofluid specific) analytical assays each with a matching set of standard deconvolution/annotation algorithms with fixed parameter settings. Conversely, other parts of the lifecycle are bespoke to the individual study; specifically, the design of experiments, data modelling, biochemical interpretation and dissemination.

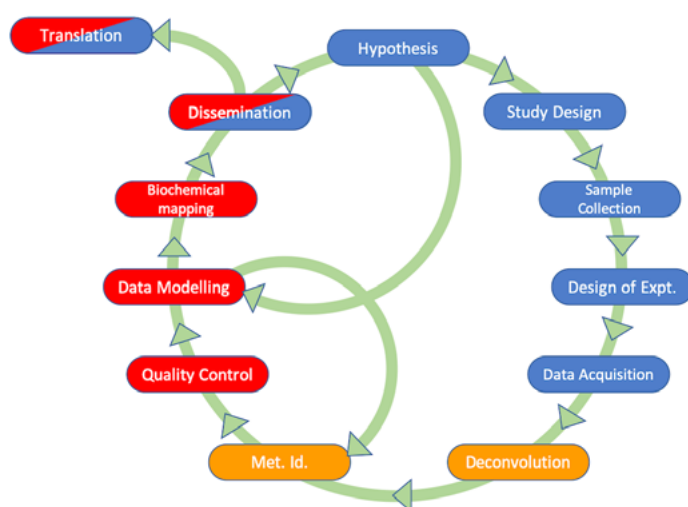


Figure 1. Lifecycle of a clinical metabolomics study

Spotlight | Jupyter Notebooks and Cloud Computing

What has this got to do with data science? Well, it is important to consider that the stages of a metabolomics lifecycle that require complex computational algorithms can be split into two distinct categories each with opposing intellectual and computational characteristics. Using vernacular taken from the artificial intelligence community, peak deconvolution, annotation and associated computational architecture can accurately be termed data engineering as the aim is to make the raw instrument data amenable to predictive modelling (e.g., disease classification) and/or biological interpretation - but no further than that. Whereas, the process of taking a curated data matrix and applying statistical, epidemiological, machine learning, visualisation techniques, together with mechanisms to translate results into biological and clinical insights can be termed data science (**Figure 2**).

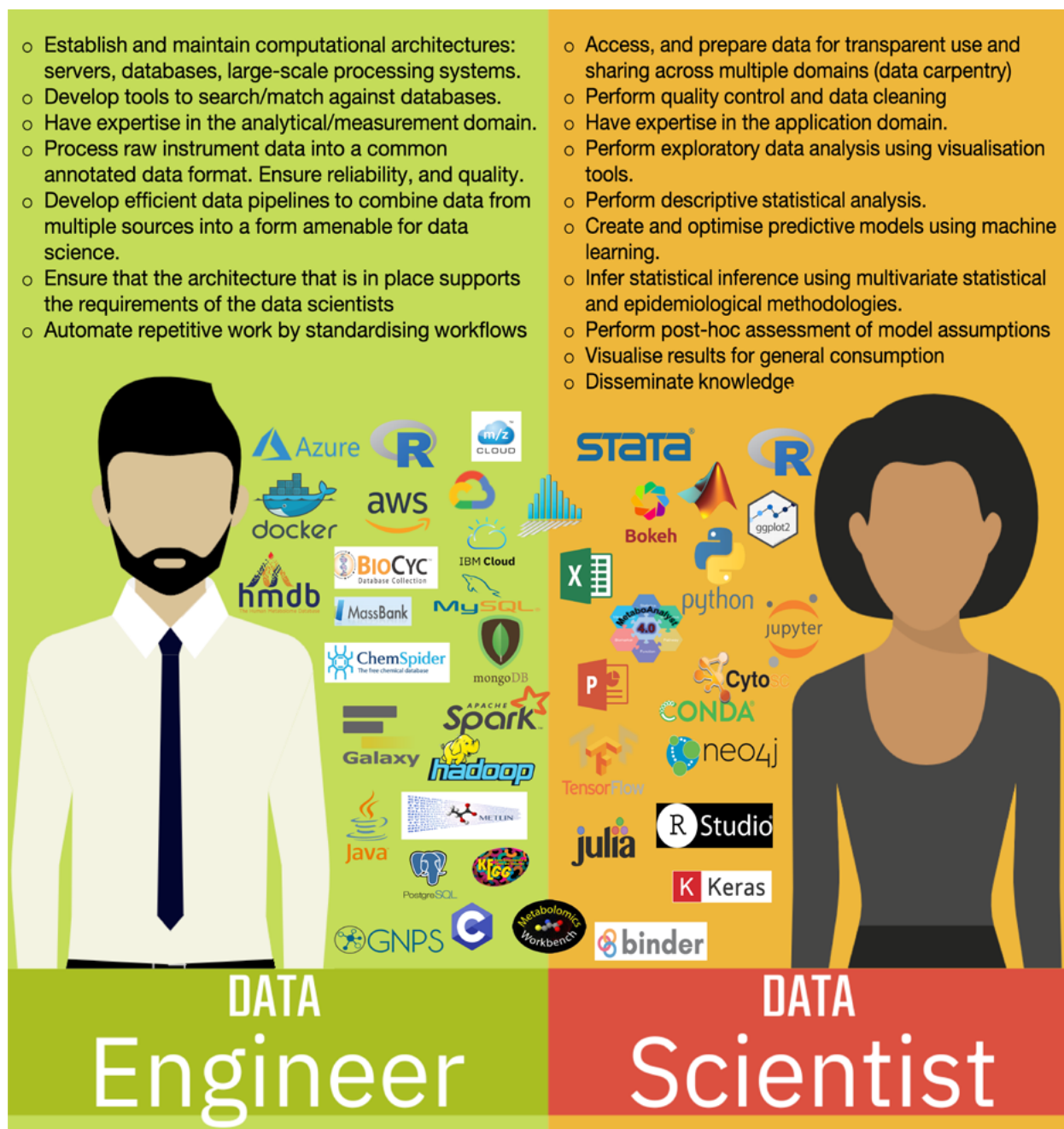
With this in mind, it would be reasonable to propose that any efforts to develop generalised computational frameworks for the metabolomics lifecycle should be approached independently with requirement specifications dependent on the specific needs of each job, and thus potentially, completely separate computational platforms. Peak deconvolution and peak annotation are computationally intensive, often taking 10s of hours to process data, but require very little interaction or creativity. They often require access to (or development of) external web services/databases and understanding of associated computational architecture. Workflows are linear and rarely change once optimised for a given lab+instrument+assay+biofluid combination (e.g., CIMCB, LC-MS, HILIC+, Urine).

As such, the underlying computational workflows take the form "design once, document once, and run many". Data modelling and visualisation, on the other hand, is computationally cheap at execution, and can be executed in an isolated (virtual) environment. Workflows require a large amount of forethought and flexibility, with potentially multiple cascading modelling workflows, each requiring cross-validated parameter optimisation, domain expertise, exploratory investigation of data structures,

post-hoc assessment of model assumptions, possibly adjusting for confounding variables or fusion with data sourced from other 'omic platforms. Each step also requires comprehensive documentation to guide reproducibility. As such, the underlying computational workflows are of the form "design many, document many, and run once".

It is also important to note that an increasing number of metabolomics researchers, particularly in the clinical domain, outsource the complete data engineering stage of the metabolomics lifecycle to a service laboratory. Companies such as Metabolon, Nightingale Health, and Biocrates have business models that depend on providing high-quality fully annotated data sets in a format amenable for data science. Most large academic laboratories also provide some sort of similar service. As such, for more and more students, academics, and industry professionals, the clinical metabolomics lifecycle is driven by data science, not by analytical chemistry, cheminformatics, or data engineering. Such approaches have most recently been reported in the American Journal of Epidemiology by Yu *et al.* (2019) "[The Consortium of Metabolomics Studies \(COMETS\) Metabolomics in 47 Prospective Cohort Studies](#)".

You may or may not agree with this perspective, but one thing that most in the metabolomics community will agree upon is the urgent need for transparent and consistent reporting of all aspects of the metabolomics study lifecycle. The metabolomics community has made substantial efforts to align with [FAIR](#) (Findable, Accessible, Interoperable, and Reusable) data principles by developing open data formats (e.g., mzXML), data repositories (e.g., [MetaboLights](#) and [Metabolomics Workbench](#)), online spectral reference (e.g., [METLIN](#), [mzCloud](#), [MassBank](#), [GNPS](#)), and online databases for metabolite identification and biochemical association (e.g., [HMDB](#)). These data engineering resources and others like them are essential to ensure the future integrity of metabolomics as a science.

Spotlight | Jupyter Notebooks and Cloud Computing**Figure 2.** Data Engineer vs. Data Scientist

Spotlight | Jupyter Notebooks and Cloud Computing

Numerous groups within the metabolomics community also actively work to standardise computational workflows and provide open source and online tools for both data engineering and data science. An excellent and comprehensive review of R packages developed for the metabolomics community has recently been published by [Stanstrup et al \(2019\)](#). That said, most attempts at a unified computational framework (e.g., Galaxy or KNIME) have primarily focussed on the requirements for data engineering, with data science forced to fit into a very prescriptive linear workflow. In our recent review for Metabolomics “[Toward collaborative open data science in metabolomics using Jupyter Notebooks and cloud computing](#)”, Mendez *et al.* (2019), we provide a brief overview of current data science programming frameworks relevant to the metabolomics community, corresponding barriers to achieving open science, and finally an introduction to one practical solution specific to data science in the form of [Jupyter Notebooks](#). Jupyter Notebooks are an open-source, web tool for creating seamless integration of text, code (typically Python or R), and outputs (tables, figures) into a single living interactive document. This framework is particularly amenable for the needs of data science. When used alongside data repositories, such as GitHub, and open cloud-based deployment services, such as Binder, these computational notebooks can greatly enhance transparent dissemination of data science methods and results during the publication process.

We provide a set of experiential learning tutorials, [hosted on the Github repository](#), introducing the Jupyter Notebook framework, specifically tailored to the needs of a metabolomics researcher with limited programming experience.

Several researchers in the metabolomics community are already using the Jupyter/Binder framework as a means for transparent dissemination for publications (e.g., [Nett et al. 2018](#); [Github](#)), or as tutorials for new data science methodologies (e.g., [AlAkwa et al. 2018](#); [GitHub Binder](#)), data engineering algorithms (e.g., [van der Hooft et al. 2016](#); [Github](#)), or both (e.g., [Sands et al. 2019](#); [Github](#), [Binder](#)). Also, it would be remiss not to link to the excellent Jupyter Notebook based [METASPACE Python-client](#).

Jupyter Notebooks may not be suitable for all metabolomics applications (particularly if the primary objective is identification of novel metabolites) and for computationally intensive data engineering it is probably not as efficient as other frameworks such as local installations of [Galaxy](#) or [KNIME](#), or dedicated commercial software such as [Compound Discover](#), [Progenesis QI](#), or [AnalyzerPro](#), or dedicated open tools such as [MS-Dial](#) and [XCMS-online](#). However, there is a desperate need for accessible and transparent reporting of data science methods and results. Jupyter Notebooks coupled with serverless cloud-computing, provides a surprisingly intuitive and rapid means of enabling transparent dissemination, open collaboration, and experiential learning.

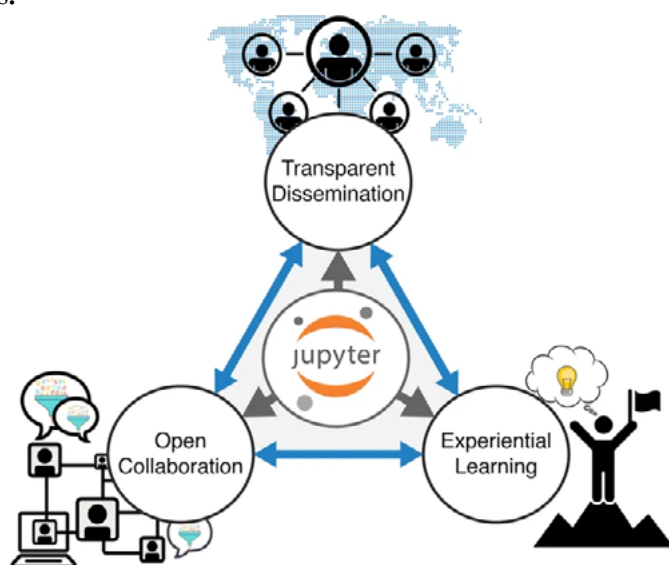


Figure 3. Taken from Mendez *et al.*, *Metabolomics* (2019)

Recent Publications

Recent Publications

Recently published papers in metabolomics

- [Using MetaboAnalyst 4.0 for Comprehensive and Integrative Metabolomics Data Analysis.](#)
- [Exposome-Explorer 2.0: an update incorporating candidate dietary biomarkers and dietary associations with cancer risk.](#)
- [Gamma-aminobutyric acid-producing lactobacilli positively affect metabolism and depressive-like behaviour in a mouse model of metabolic syndrome.](#)
- [Cheminformatics and Computational Approaches in Metabolomics.](#)
- [Untargeted metabolomic analysis of plasma from relapsing-remitting multiple sclerosis patients reveals changes in metabolites associated with neurocognitive and structural changes in brain.](#)
- [Applications of stable isotope-based metabolomics and fluxomics toward synthetic biology of cyanobacteria.](#)
- [Accessible and reproducible mass spectrometry imaging data analysis in Galaxy.](#)
- [Bioenergetics and translational metabolism: implications for genetics, physiology and precision medicine.](#)
- [Plasma metabolite biomarkers of boiled and filtered coffee intake and their association with type 2 diabetes risk.](#)
- [Pathway Tools version 23.0 update: software for pathway/genome informatics and systems biology.](#)



Metabolomics Events

22-24 January 2020

European RFMF Metabomeeting

Venue:

Toulouse, France

Overview

The French-speaking Metabolomics and Fluxomics Network (RFMF), Metabolomics Profiling Forum (MPF, Metabomeeting) and European regional metabolomics networks are pleased to announce a joint conference taking place from 22nd to 24th January 2020 in Toulouse (France).

The European RFMF Metabomeeting in Toulouse will propose thematic sessions dedicated to:

- Analytical developments in Metabolomics & Fluxomics
- Computational and statistical developments in Metabolomics & Fluxomics
- Cutting edge applications of Metabolomics and Fluxomics in:
 - Human health
 - Agriculture & Food
 - Environmental science
 - Microbiology & biotechnologies

<https://rfmf-mpf-2020.sciencesconf.org>

3-7 February 2020

Workflow4Experimenters International Course

Venue:

Brussels, Belgium

Overview

The French Institute of Bioinformatics (IFB, Elixir-FR) and the Infrastructure for Metabolomics and Fluxomics (MetaboHUB) organize in collaboration with the Université libre de Bruxelles the next **Workflow4Experimenters International Course** (W4E2020).

Analyze your own data with Galaxy and the Workflow4metabolomics e-infrastructure! The next Workflow4Experimenters international course (W4E2020) will take place in Brussels (February 3 to February 7, 2020). During this one-week course (entirely in English), you will learn how to use Galaxy and the W4M infrastructure to analyze your own LC-MS, GC-MS, or NMR data set. Morning sessions will be dedicated to methodology and tools. Afternoon sessions will be devoted to tutoring.

Metabolomics Events

Invited speakers: Dr. S. Marr (Leibniz Institute of Plant Biochemistry, Germany), Dr. R. Weber (Phenome Centre Birmingham, United Kingdom), Dr. N. Poupin (Unité Toxalim, INRA Toulouse, France)

Registrations: <https://workflow4metabolomics.org/w4e2020>

Contact: contact@workflow4metabolomics.org



10-12 Feb & 23-25 Sep 2020

Multiple Biofluid and Tissue Types, From Sample Preparation to Analysis Strategies for Metabolomics

Venue:

Birmingham Metabolomics Training Centre, University of Birmingham, United Kingdom

Overview

This 3-day course provides a theoretical overview and hands-on training to apply multiple sample preparation and UPLC-MS methods to characterise the metabolomes of complex biological samples using the mass spectrometer (Xevo QToF G2-XS - a maximum of 4 people working on the instrument in a session). The course is led by experts in the field who have experience of the analysis of microbial, plant and mammalian samples, and illustrates the different approaches that are available to analyse a range of biological samples and applying complementary liquid chromatography approaches to maximise the coverage of the metabolome.

Topics Covered

- Introduction to dealing with the complexity of biological samples using UPLC-MS
- Overview of different sample collection, sample quenching and sample extraction methods
- The challenges of working with cellular and tissue samples
- Overview of different UPLC methods including HILIC and reversed phase methods
- Hands-on sample preparation of plasma, urine, cell and tissue samples
- Monophasic and biphasic solvent extraction methods to target polar and non-polar metabolites
- SPE and liquid-liquid sample clean-up methods
- Hands-on HILIC and reversed-phase liquid chromatography
- Hands-on UPLC-MS analysis for untargeted studies (maximum of 4 people)
- Overview of data analysis and metabolite identification
- Problem solving and tips and tricks session with the experts

Course Links:

February 2020

<https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/2020/Multiple-biofluid-and-tissue-types-from-sample-preparation-to-analysis-strategies-for-metabolomics-February-2020.aspx>

September 2020

<https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/2020/Multiple-biofluid-and-tissue-types-from-sample-preparation-to-analysis-strategies-for-metabolomics-September-2020.aspx>

Metabolomics Events

14 February 2020

Human Brain Project & Dutch Neuroscience: Shaping Collaborations

Venue:

Pakhuis De Zwijger, Amsterdam

Overview

The world's first integrated ICT infrastructure for brain research and development: What could you do with EBRAINS? [View details here.](#)

30 Mar - 1 Apr 2020

Metabolomics with the Q Exactive

Venue:

Birmingham Metabolomics Training Centre, University of Birmingham, United Kingdom

Overview

This 3-day course introduces you to using the Q Exactive mass spectrometer in your metabolomics investigations. The course is led by experts in the field of metabolomics and includes lectures, laboratory sessions and computer workshops to provide a detailed overview of the metabolomics pipeline applying the Q Exactive mass spectrometer.

Topics Covered

- Introduction to Metabolomics on the Q Exactive, the metabolomics workflow, and case studies using the Q Exactive
- Using the Q Exactive family of instruments in your metabolomics investigations
- Experimental design and the importance of quality control samples
- Sample preparation including polar and non-polar preparation methods on biofluids (urine and plasma) and tissue samples
- Preparation of samples for profiling and targeted analyses on the Q Exactive
- Hands-on data acquisition for profiling and targeted studies, setting up the Vanquish UHPLC coupled to the Q Exactive MS
- Data processing workshop
- Data analysis workshop (univariate and multivariate analysis)
- Introduction to metabolite identification applying Data Dependent Analysis and Data Independent Analysis
- Question and answer session with a panel of experts
- Tips and tricks
- Problem solving

Course link:

<https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/2020/Metabolomics-with-the-Q-Exactive-April-2020.aspx>

Metabolomics Events

30 Mar - 2 Apr 2020

Introduction to Metabolomics Analysis

Venue:

European Bioinformatics Institute (EMBL-EBI) - Wellcome Genome Campus, Hinxton, Cambridge, CB10 1SD, United Kingdom

Overview

Application opens: Monday 23 September 2019

Application deadline: Friday 29 November 2019

Participation: Open application with selection

Contact: Meredith Willmott

Registration fee: £650 - Including meals and accommodation

Learn more at <https://www.ebi.ac.uk/training/events/2020/introduction-metabolomics-analysis-1>



2-3 April 2020

Metabolite identification with the Q Exactive and LTQ Orbitrap

Venue:

Birmingham Metabolomics Training Centre, School of Biosciences, University of Birmingham, Birmingham, UK

Overview

This two-day course will provide a hands-on approach to teach the attendees about the latest techniques and tools available to perform metabolite identification in non-targeted metabolomics studies. The course will be led by experts working within the fields of metabolomics and chemical analysis and will include a significant proportion of hands-on experience of using mass spectrometers, software tools and databases. A maximum of four people will be working on each mass spectrometer in a session. We will apply these tools on the Q Exactive and LTQ-Orbitrap family of mass spectrometers.

Topics Covered

- Importance of mass spectral interpretation
- Types of data which can be collected on the QE and LTQ-Orbitrap (m/z, retention time, MS/MS, MSn)
- Conversion of raw data to molecular formula and putative metabolite annotations
- MS/MS experiments in metabolic phenotyping for on-line data acquisition using the QE (DDA, DIA, all-ion)
- MS/MS and MSn experiments for sample fractions using the LTQ-Orbitrap
- Mass spectral libraries (using mzCloud)
- Searching mass spectral libraries
- Tools for mass spectral interpretation
- Reporting standards for metabolite identification
- Question and answer session with the experts

Course link: <https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/metabolite-identification.aspx>

Metabolomics Events



27-29 April & 7-9 Oct 2020

Introduction to Metabolomics for the Microbiologist

Venue:

Birmingham Metabolomics Training Centre, School of Biosciences, University of Birmingham, Birmingham, UK

Overview

This three-day course introduces how untargeted metabolomics can be applied to study microbial systems in academic and industrial research. The course provides an overview of the metabolomics pipeline, experimental design, sample preparation and data acquisition. The course is led by experts in the field of metabolomics and will include lectures, hands-on laboratory sessions in sample preparation and data acquisition and computer workshops focused on data processing and data analysis.

Topics Covered

- Introduction to metabolomics, both targeted and untargeted approaches
- Experimental design and the importance of quality control samples in untargeted metabolomics
- Analytical strategies applied in metabolomics with a focus on mass spectrometry
- Hands-on laboratory sessions focused on sample preparation and to include metabolic quenching and extraction procedures, intracellular and exometabolome samples and polar and non-polar extraction methods
- Hands-on laboratory sessions focused on sample analysis for untargeted metabolomics studies using an Acquity UPLC coupled to a Xevo QToF mass spectrometer
- Hands-on workshop focused on data processing and data analysis
- Hands-on workshop focused on an introduction to metabolite identification
- Question and answer session with the experts

Course Link:

April 2020

<https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/2020/Introduction-to-Metabolomics-for-the-Microbiologist-April-2020.aspx>

October 2020

<https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/2020/Introduction-to-Metabolomics-for-the-Microbiologist-October-2020.aspx>



6-10 July 2020

Metabolomics 2020

Venue:

Shanghai, China

Overview

The 16th Annual International Conference of the Metabolomics Society will be held in Shanghai, China from July 6-10, 2020.

Check back for updates in the coming months at <http://metabolomics2020.org>.

Metabolomics Events



2-4 Nov 2019

Metabolomics with the Q Exactive

Venue:

Birmingham Metabolomics Training Centre, School of Biosciences, University of Birmingham, Birmingham, UK

Overview

This three-day course introduces you to using the Q Exactive mass spectrometer in your metabolomics investigations. The course is led by experts in the field of metabolomics and includes lectures, laboratory sessions and computer workshops to provide a detailed overview of the metabolomics pipeline applying the Q Exactive mass spectrometer.

Topics Covered

- Introduction to Metabolomics on the Q Exactive, the metabolomics workflow, and case studies using the Q Exactive
- Using the Q Exactive family of instruments in your metabolomics investigations
- Experimental design and the importance of quality control samples
- Sample preparation including polar and non-polar preparation methods on biofluids (urine and plasma) and tissue samples
- Preparation of samples for profiling and targeted analyses on the Q Exactive
- Hands-on data acquisition for profiling and targeted studies, setting up the Vanquish UHPLC coupled to the Q Exactive MS
- Data processing workshop
- Data analysis workshop (univariate and multivariate analysis)
- Introduction to metabolite identification applying Data Dependent Analysis and Data Independent Analysis
- Question and answer session with a panel of experts
 - Tips and Tricks
 - Problem Solving

Course link:

<https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/2020/Metabolomics-with-the-Q-Exactive-November-2020.aspx>



5-6 November 2019

Metabolite identification with the Q Exactive and LTQ Orbitrap

Venue:

Birmingham Metabolomics Training Centre, School of Biosciences, University of Birmingham, Birmingham, UK

Overview

This two-day course will provide a hands-on approach to teach the attendees about the latest techniques and tools available to perform metabolite identification in non-targeted metabolomics studies. The course will be led by experts working within the fields of metabolomics and chemical analysis and will include a significant proportion of hands-on experience of using mass spectrometers, software tools and databases. A maximum of four people will be working on each mass spectrometer in a session. We will apply these tools on the Q Exactive and LTQ-Orbitrap family of mass spectrometers.

Metabolomics Events

Topics Covered

- Importance of mass spectral interpretation
- Types of data which can be collected on the QE and LTQ-Orbitrap (m/z, retention time, MS/MS, MS_n)
- Conversion of raw data to molecular formula and putative metabolite annotations
- MS/MS experiments in metabolic phenotyping for on-line data acquisition using the QE (DDA, DIA, all-ion)
- MS/MS and MS_n experiments for sample fractions using the LTQ-Orbitrap
- Mass spectral libraries (using mzCloud)
- Searching mass spectral libraries
- Tools for mass spectral interpretation
- Reporting standards for metabolite identification
- Question and answer session with the experts

Course link:

<https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/2020/Metabolite-identification-with-the-Q-Exactive-and-LTQ-Orbitrap-Elite-November-2020.aspx>

Metabolomics Jobs

Metabolomics Jobs & Collaborations

If you have a job you would like posted, please email Ian Forsythe (metabolomics.innovation@gmail.com).

Jobs Offered

Job Title	Employer	Location	Posted	Closes	Source
Various positions			9-Dec-19		Metabolomics Association of North America Jobs
Postdoctoral position in Dr. Andres-Lacueva's group	University of Barcelona	Barcelona, Spain	5-Dec-19	Until filled	Metabolomics Society Jobs
Postdoctoral Fellow in Metabolomics	Wake Forest University Health Sciences	Winston-Salem, NC, USA	20-Nov-19	Until filled	Metabolomics Society Jobs
Director Business Development - Home Based in the US	Biocrates Life Sciences	US based	10-Oct-19	Until filled	Metabolomics Society Jobs
Business Development Manager - Home Based in the USA	Biocrates Life Sciences	US based	10-Oct-19	Until filled	Metabolomics Society Jobs
Postdoctoral Researcher Position Microbial Metabolomics	Friedrich Schiller University Jena	Jena, Germany	7-Oct-19		Friedrich Schiller University Jena
Assistant Research Professor	Penn State University	University Park, PA, USA	23-Sep-19	Until filled	Metabolomics Society Jobs
Postdoctoral Fellow, GC-MS Metabolomics	Wake Forest University Health Sciences	Winston-Salem, NC, USA	7-Sep-19	Until filled	Wake Forest University Health Sciences

Metabolomics Jobs

Jobs Wanted

This section is intended for very highly qualified individuals (e.g., lab managers, professors, directors, executives with extensive experience) who are seeking employment in metabolomics.

We encourage these individuals to submit their position requests to Ian Forsythe (metabolomics.innovation@gmail.com). Upon review, a limited number of job submissions will be selected for publication in the Jobs Wanted section.

- [Seeking New Challenges in Metabolomics](#)
-