MetaboNews

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

Metabolomics Society News

Members Corner

Early-Career Members Network (EMN)

The EMN Webinar Series 2019

EMN webinar was held on April 23rd (3 pm PST, 5 pm CST, 6 pm EST, 11 pm GMT), 24th (12:00 am CET, 7 am China Time, 8 am Japan Time, 10 am AEDT) 2019. Dr Hiroshi Tsugawa from RIKEN institute, Japan discussed computational mass spectrometry in metabolomics to deepen the understanding of metabolisms. He also introduced three computational software packages (MS-DIAL, MS-FINDER and MRMPROBS) supporting metabolomics data analysis.

You can access the recorded videos of past webinars on the Metabolomics Society website. Please stay tuned and look out for the next EMN webinar series session.

EMN Travel Bursary Grant 2019: Evaluation Ongoing
We have received over 40 applications and are looking forward to announcing the winners after the evaluation. Results will also be posted on Twitter and Facebook!

EMN Workshops at Metabolomics 2019
Save the date for EMN workshops on June 23-24, 2019, at The Hague, The Netherlands. This year, we will host several workshop sessions tailored for the needs of early-career scientists who are new to metabolomics. If you attend the conference, please join us! For more detail, please check the website.

New to metabolomics or stuck with a problem? We recommend Metabolomics wiki and Metabolomics Forum. Follow us on Twitter (@MetabolomicsSoc) and Facebook (@EMN.metabolomicssociety) to stay up-to-date on all news and upcoming events.

METABOLOMICS SOCIETY

METABOLOMICS SOCIETY
EARLY- CAREER MEMBERS NETWORK

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

General Enquiries
info@metabolomicssociety.org

Task Group Corner

Industry Engagement Task Group

An email went out to all Society members in January 2019, to encourage participation in the reinvigoration of the Industry Engagement Task Group (ITG). Thirty-three members showed interested in participating and twelve were able to attend our first meeting on February 20, 2019. Based on decisions made at the February 20, 2019 meeting, the ITG will have a leadership structure of two Co-Chairs plus one Board of Directors member and will allow a maximum of 12 "standing" members, who are elected to a one-year term. Standing members can commit to attending 10 out of 12 meetings per year. The ITG will also conduct bi-annual, online meetings for all interested parties to attend. Potentially we will meet as well at the annual Metabolomics Society meeting.

We are pleased to announce the results of voting and congratulate our 2019 Co-Chairs and "standing" members (elected to a one-year- term): Rob Vreeken and Fadi Abdi (Co-Chairs with Nichole Reisdorph representing the BOD), Jerzy (Jurek) Adamski, Georgia Charkoftaki, Melissa Fitzgerald, Heino Heyman, David Heywood, Doris Jacobs, and Tytus Mac (Standing members). Please see the website for the full list, including affiliations.

The ITG will meet once per month and are already defining goals for the next several months. If you have questions or would like to receive ITG updates, please contact Nichole Reisdorph (Nichole.Reisdorph@ucdenver.edu), Fadi Abdi, (fadi.abdi@Biocrates.com) or Rob Vrkeeken (rvreeken@its.jnj.com). We look forward to bringing you more updates soon!

SpOtlight

The Virtual Metabolic Human Database

Mapping the metabolome onto human and gut microbial metabolism, human diseases and nutrition

Cyrille C. Thinnes and Ines Thiele

Luxembourg Centre for Systems Biomedicine, University of Luxembourg

Human physiology is intricately connected to the metabolome, governed by the dynamic and context-dependent interplay on a cellular and organismal level between the human, the microbiome, nutrition, life style, and associated health status. Metabolomics provides information on the immediate metabolic phenotype and can directly reflect the consequences of health status, which makes the analysis of metabolomic data particularly valuable for biomedical research. However, metabolomic profiles still remain difficult to analyze in the overall biochemical context, limiting the interpretation to potential altered metabolic pathways rather than providing a comprehensive understanding of the underlying mechanistic basis.

This shortcoming can be addressed with the biochemically well-defined framework of genome-scale metabolic reconstructions, which are assembled in a bottom-up manner based on genomic, biochemical, and physiological data. As such, genome-scale metabolic reconstructions allow for a high-dimensional data analysis and can provide novel insights into the mechanisms underlying observed differences in the metabolome, e.g., in health and disease. Moreover, the study of complex and multifactorial systems for, e.g., advancing precision medicine and personalized nutrition, benefits from efficient computational systems approaches.

To facilitate the integrative analysis of metabolomic data in their biochemical context, we developed a novel database, the Virtual Metabolic Human (VMH, www.vmh.life). The VMH hosts and interlinks the human and associated gut microbe metabolic reconstructions with an extensive nutrition database and hundreds of metabolic diseases using standardized nomenclature (DOI: 10.1093/nar/gky992). Extensive manual curation protocols enabled the high standard and information coverage of the VMH-hosted genome-scale metabolic reconstructions, i.e., the complete computational representation, for both human and associated microbes, of known metabolism in relations to the underlying gene, protein, and biochemical networks.

The VMH currently captures 5,180 unique metabolites, 17,730 unique reactions, 3,695 human genes, 255 Mendelian diseases, 818 microbes, 632,685 microbial genes, and 8,790 food items. Importantly, the metabolite entities are associated with 22 database-dependent and -independent entities (Figure 1) as well as with metabolite structures and thermochemical estimates (e.g., standard Gibbs free energy). Moreover, the VMH lists biochemical reactions, in which a metabolite participates in along with predicted atom mappings, a valuable entry point for the identification of conserved moieties in metabolism and simulation of isotope labeling experiments.

In total, the VMH connects its entities to 57 other web resources making it an ideal starting point for biochemical and biomedical research.

Computational models can be generated from the genome-scale metabolic reconstructions contained in the VMH using condition-specific information, such as metabolomic or transcriptomic data, and appropriate computational toolboxes, such as the open-access community-driven Constraint-Based Reconstruction and Analysis (COBRA) Toolbox. The generated in silico metabolic models enable the formulation of novel mechanism-based hypotheses for a variety of biomedical and biotechnological challenges. In this context, the VMH Diet Designer is particularly helpful to propose personalized diets for assessing individual subgroups or nutrition-based interventions.

Click Above: VMH QuickStart tutorial, as an example of the VMH tutorial series

Consequently, the VMH has been at the basis of several biomedical studies, including those with focus on Parkinson's disease (DOI: 10.1038/npjsba.2016.13) or irritable bowel disease (DOI: 10.1101/229138). Crucially, the VMH has been instrumental for the generation of the first physiologically accurate, organ-resolved mechanistic models of whole-body metabolism, interlinked with microbiome-level metabolic models (DOI: 10.1101/255885). Integrating an individual's physiological, biochemical, metabolomic, and (meta) genomic data, this new generation of computational models represents a pivotal step towards personalized, predictive modeling for enabling personalized medicine and personalized nutrition.

The central and interconnected design of the VMH allows for the visualization of metabolic networks on the VMH's Google-like metabolic maps: ReconMaps (Figure 1D). Supporting open science, the VMH is freely accessible to the research community via the website and application-programming interface (API) to query and download its content.

Beyond making the scientific content available, the VMH team strives to engage the research community by continuously incorporating user feedback on improvements, providing tutorials, organizing hands-on workshops, and holding reconstruction jamborees. In summary, the VMH provides a novel, interdisciplinary research tool by increasing the availability of diverse data and knowledge along the diet-gut-health axis to the biomedical and metabolomic communities.

Figure 1 overleaf:

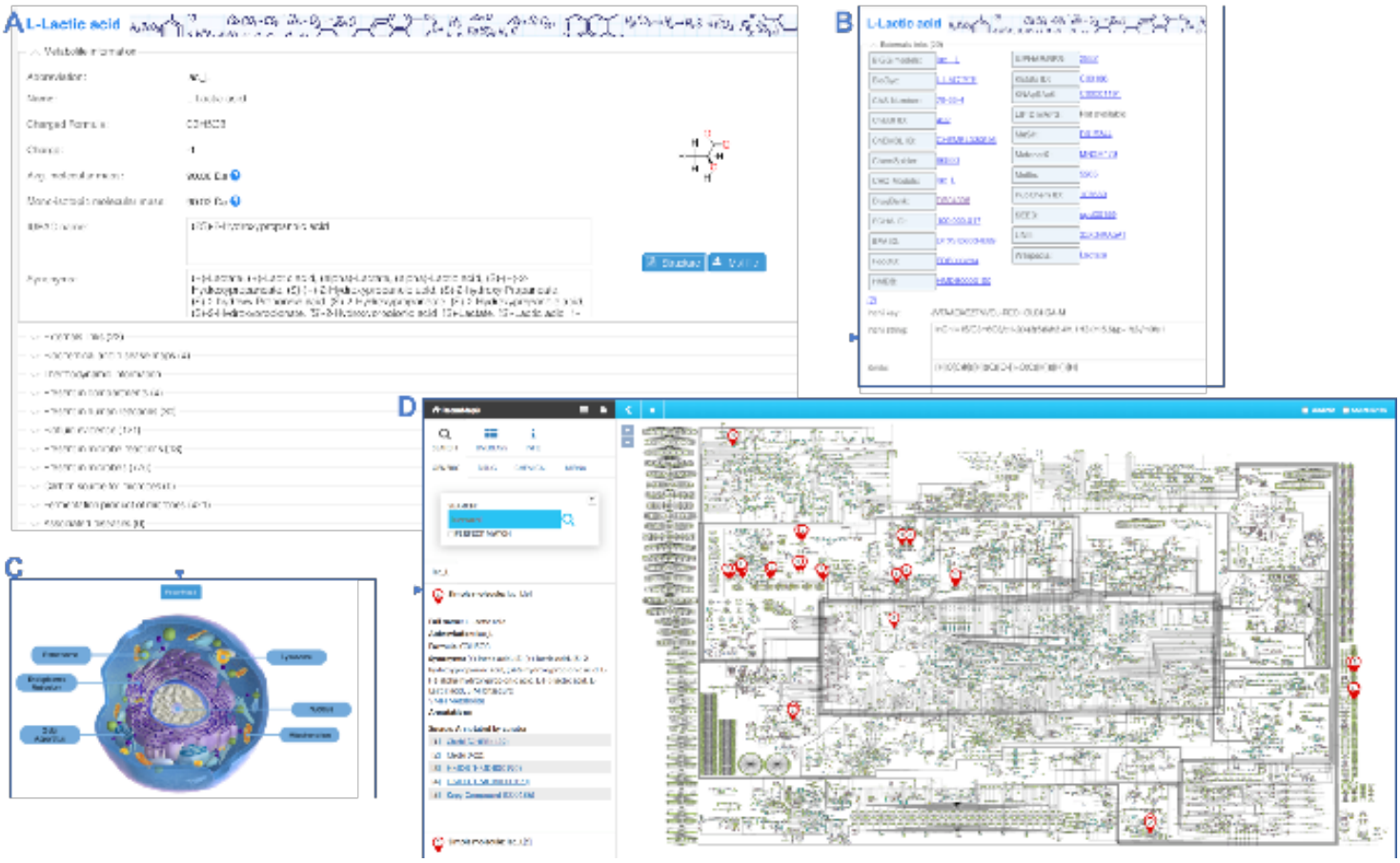


Figure 1: Putting metabolites into their metabolic context using the Virtual Metabolic Human database (VMH, www.vmh.life). **A.** Metabolite page for L-lactic acid (VMH ID: lac_L). Detailed information about the metabolite is provided as well as internal and external links. Each metabolite has one or more metabolic reactions associated in human and/or microbial metabolism. Furthermore, the VMH provides information whether the metabolite has been identified in human biofluids, whether the metabolite is a carbon source or fermentation product for the gut microbes, and whether diseases have been associated with a metabolite. All information was manually assembled and literature references are provided in the corresponding internal pages, if available. **B.** Each metabolite entry in the VMH links to 19 external reference databases and three database-independent identifiers are provided. Importantly, the VMH database may be queried using any of these identifiers, enabling easy access to its metabolite content. **C.** The VMH contains a set of seven manually drawn Google-like metabolic maps, capturing the metabolism occurring in six organelles as well as one comprehensive overview map (ReconMap3). **D.** Metabolite(s) may be put visually into their metabolic context using, for example, the ReconMap3, which covers thousands of human metabolic reactions. Similarly, metabolomic data may be mapped onto the ReconMap3 as well as computational simulation results, using the tutorial provided in the COBRA Toolbox.

Recent Publications

Recently published papers in metabolomics

- Chemical Composition of Commercial Cow's Milk
- Combined hydrophilic interaction liquid chromatography-scanning field asymmetric waveform ion mobility spectrometry-time-of-flight mass spectrometry for untargeted metabolomics
- The Type 2 Diabetes Susceptibility PROX1 Gene Variants Are Associated with Postprandial Plasma Metabolites Profile in Non-Diabetic Men
- Potential Nutritional and Metabolomic Advantages of High Fat Oral Supplementation in Pancreatectomized Pancreaticobiliary Cancer Patients
- Untargeted LC/MS-based metabolic phenotyping (metabonomics/metabolomics): The state of the art
- A Pilot Metabolomics Study of Tuberculosis Immune Reconstitution Inflammatory Syndrome
- Rapid profiling of triglycerides in human breast milk using LESA-FTMS reveals new VLCFAs and differences within individuals
- Metabolomics-Based Biosignatures of Prostate Cancer in Patients Following Radiotherapy
- Time of Exercise Specifies the Impact on Muscle Metabolic Pathways and Systemic Energy Homeostasis
- A gas chromatography-mass spectrometry untargeted metabolomics approach to discriminate Fiore Sardo cheese produced from raw or thermized ovine milk

Metabolomics Events

1-2 May 2019

The Second Annual Canadian Metabolomics Conference

Venue:
Coast Canmore Hotel & Conference Centre, Canmore, Alberta, Canada

Overview
The Second Annual Canadian Metabolomics Conference will be held from May 1st to 2nd in Canmore, Alberta. The conference will highlight work by leading researchers, including new technologies and approaches for metabolomics research, and applications in various fields. The conference will feature networking opportunities and a poster session designed for trainees to present their work. The Alberta Epigenetics Network will be offering trainee travel awards. Our goal is to highlight the exceptional metabolomics science that is being done in Canada and abroad, and foster Canada's leadership role in the global research community.

We look forward to seeing you in beautiful Canmore, Alberta.

Conference links:
- Program: https://www.canmetcon.ca/program
- Registration: https://www.canmetcon.ca/registration
- Abstract Submission: https://www.canmetcon.ca/abstract-submission

For further details, please visit https://www.canmetcon.ca/

Metabolomics Events

13-15 May 2019

Challenges in Analysis of Complex Natural Mixtures Faraday Discussion

Venue:
John McIntyre Conference Centre, University of Edinburgh, 18 Holyrood Park Road, Edinburgh, EH16 5AY, United Kingdom

Overview

Structure determination of molecules contained within unresolved complex mixtures represents an unsolved question that continues to challenge physical and analytical chemistry. Most naturally occurring systems can be characterised as complex mixtures. These can be broadly divided according to the molecular sizes of their constituents, into mixtures of small or large molecules. The focus of this Faraday Discussion will be on the former, while the latter such as biomacromolecules, industrial polymers, or solid matrices are outside of its scope as such. Nevertheless, the processes that are used in analysing the data originating from these studies may be of interest.

Examples of small molecule mixtures include:

- Environmental matrices such as soil, dissolved organic matter, organic molecules contained in atmospheric aerosol particles, or crude oil
- Biofluids
- Man-made mixtures of small molecules such as food, beverages or plant extracts

These systems are generally classed as “complex mixtures” or “unresolved complex mixtures (UCM)”, emphasising our current inability to separate their individual components.

The techniques best positioned to tackle such mixtures experimentally include mass spectrometry, chromatography, NMR spectroscopy, or new alternative techniques, including combinations of the above methods. For the most part, people who work on the analysis of complex mixtures are driving the progress in exploiting new methodologies and their creative combinations.

For further information and registration details, please visit http://www.rsc.org/events/detail/29574/challenges-in-analysis-of-complex-natural-mixtures-faraday-discussion

13 May - 7 June 2019

Metabolomics: Understanding Metabolism in the 21st Century

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

Overview

Metabolomics is an emerging field that aims to measure the complement of metabolites (the metabolome) in living organisms. The metabolome represents the downstream effect of an organism’s genome and its interaction with the environment. Metabolomics has a wide application area across the medical and biological sciences. The course provides an introduction to metabolomics, describes the tools and techniques we use to study the metabolome and explains why we want to study it. By the end of the course you will understand how metabolomics can revolutionise our understanding of metabolism.

Metabolomics Events

Topics Covered

- Metabolism and the interaction of the metabolome with the genome, proteome and the environment
- The advantages of studying the metabolome
- The application of hypothesis generating studies versus the use of traditional hypothesis directed research
- The use of targeted and non-targeted studies in metabolomics
- An interdisciplinary approach with case-studies from clinical and environmental scientific areas
- Important considerations in studying the metabolome
- Experimental design and sample preparation
- The application of mass spectrometry in metabolomics
- An introduction to data processing and analysis
- Metabolite identification

Course link:
https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/Metabolomics-MOOC.aspx

16-17 May 2019

5th Workshop on Analytical Metabolomics

Venue:

Aristotle University Research Dissemination Center and Central Library, Aristotle University Campus, Thessaloniki, Greece

Overview

With great pleasure we invite you to the 5th Metabolomics Workshop to be held in Thessaloniki, Greece from 16-17 May 2019.

In addition to the workshop this year we plan three days hands-on workshop from 13-15 May in our new state of the art laboratory facility. The hands-on course will host up to 12 researchers and cover experimental design, sample preparation, LC-MS analysis, GC-MS analysis, data mining, statistics. Participants for the hand-on course will be selected on first-come, first-served basis.

The meeting is the continuation of successful meetings that started in Thessaloniki in 2008 and 2016, Athens in 2012 and Patras in 2014.
Past meetings featured renown invited speakers from academia, industry and the regulators advocating and debating on the application of holistic analytical approaches in biomarker discovery in life, plant and food sciences. We intend to bring the same high level of lectures to further promote knowledge on this upcoming field.

The potential and the benefits of applying metabolomics in life and plant/food/nutrition sciences will be the focus of the workshop.
Developments on analytical methods, data treatment strategies and tools will also be illustrated Selected software could be shown in live action. The scope is to generate discussion and interaction among the participants. Presentation options are as either oral or poster mode.

For further information and registration details, please visit:
http://biomic.web.auth.gr/workshop2019/

Metabolomics Events

27-28 May 2019

Informatics and Statistics for Metabolomics

Venue:
Edmonton, Alberta, Canada

Overview

Using high-throughput technologies, life science researchers can identify and characterize all the small molecules or metabolites in a given cell, tissue, or organism. The CBW course covers many topics ranging from understanding metabolomics technologies, data collection and analysis, using pathway databases, performing pathway analysis, conducting univariate and multivariate statistics, working with metabolomic databases, and exploring chemical databases. Hands-on practical tutorials using various data sets and tools will assist participants in learning metabolomics analysis techniques.

Participants will gain practical experience and skills to be able to:

- Design appropriate metabolome-focused experiments
- Understand the advantages and limitations of metabolomic data analysis
- Devise an appropriate bioinformatics workflow for processing and analyzing metabolomic data
- Apply appropriate statistics to undertake rigorous data analysis
- Visualize datasets to gain intuitive insights into the composition and/or activity of their metabolome

For more information, please visit https://bioinformatics.ca/workshops/informatics-and-statistics-for-metabolomics/

Metabolomics Events

16-20 September 2019

The EMBO Practical Course "Metabolomics Bioinformatics in Human Health"

Venue:
The International Agency for Research on Cancer (IARC), Lyon, France

Application Deadline:
April 15. 2019

Registration:
https://training.iarc.fr/embo-practical-course-metabolomics-bioinformatics-in-human-health/

Overview

The EMBO Practical Course "Metabolomics Bioinformatics in Human Health" will be held in the International Agency for Research on Cancer on September 16-20, 2019 and will provide an advanced overview with hands-on practical on key issues and challenges in metabolomics, handling datasets and procedures for the analysis of metabolomics data using bioinformatics tools. Combining lectures from experts, computer-based practical sessions and interactive discussions, the EMBO Practical Course will provide a platform for discussion of the key questions and challenges in this field, from study design to metabolite identification.

This five-day course is aimed at PhD students, post-docs and researchers with at least one to two years of experience in the field of metabolomics who are seeking to improve their skills in metabolomics data analysis. Participants ideally must have working experience using R (including a basic understanding of the syntax and ability to manipulate objects).

During this course you will learn about:

- Metabolomics study design, QC, workflows and sources of experimental error, targeted and untargeted approaches
- Metabolomics data processing tools: **hands on open source** R based programs, XCMS, MetFrag, and MetFusion
- NMR and Computer-assisted structure elucidation
- Metabolomics data analysis: Using R Bioconductor, understanding usage of univariate and multivariate data analysis, data fusion concepts, data clustering, machine learning and regression methods
- Metabolomics downstream analyses: KEGG, BioCyc, and MetExplore for metabolic pathway and network analysis with visualisation of differential expression, understanding metabolomics flux analysis

International Agency for Research on Cancer

World Health Organization

Metabolomics Events

23 Sept - 18 Oct 2019

Metabolomics: Understanding Metabolism in the 21st Century

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

Overview
Metabolomics is an emerging field that aims to measure the complement of metabolites (the metabolome) in living organisms. The metabolome represents the downstream effect of an organism's genome and its interaction with the environment. Metabolomics has a wide application area across the medical and biological sciences. The course provides an introduction to metabolomics, describes the tools and techniques we use to study the metabolome and explains why we want to study it. By the end of the course you will understand how metabolomics can revolutionise our understanding of metabolism.

Topics Covered
- Metabolism and the interaction of the metabolome with the genome, proteome and the environment
- The advantages of studying the metabolome
- The application of hypothesis generating studies versus the use of traditional hypothesis directed research
- The use of targeted and non-targeted studies in metabolomics
- An interdisciplinary approach with case-studies from clinical and environmental scientific areas
- Important considerations in studying the metabolome
- Experimental design and sample preparation
- The application of mass spectrometry in metabolomics
- An introduction to data processing and analysis
- Metabolite identification

Course link:
https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/Metabolomics-MOOC.aspx

25-27 Sep 2019

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

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

Overview
This three-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.

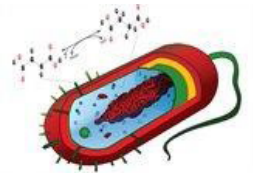
Metabolomics Events

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 link: https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/sample-analysis.aspx

BIRMINGHAM METABOLOMICS TRAINING CENTRE



9-11 Oct 2019

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: https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/introduction-metabolomics-microbiologist.aspx

Metabolomics Events

21 Oct - 15 Nov 2019

Metabolomics Data Processing and Data Analysis

Venue:
The University of Florida Clinical & Translational Science Institute, Gainesville, Florida USA

Overview
This online course explores the tools and approaches that are used to process and analyse metabolomics data. You will investigate the challenges that are typically encountered in the analysis of metabolomics data, and provide solutions to overcome these problems. The course is delivered using a combination of short videos, articles, discussions, and online workshops with step-by-step instructions and test data sets. We provide quizzes, polls and peer review exercises each week, so that you can review your learning throughout the course.

The material is delivered over a four-week period, with an estimated learning time of four hours per week. We support your learning via social discussions where you will be able post questions and comments to the team of educators and the other learners on the course. In the final week of the course there is a live question and answer session with the entire team of educators. If you do not have time to complete the course during the 4-week period you will retain access to the course material to revisit, as you are able.

Topics Covered
- An introduction to metabolomics
- An overview of the untargeted metabolomics workflow
- The influence of experimental design and data acquisition on data analysis and data quality
- Processing of NMR data
- Processing direct infusion mass spectrometry data
- Processing liquid chromatography-mass spectrometry data
- Reporting standards and data repositories
- Data analysis, detecting outliers and drift, and pre-treatment methods
- Univariate data analysis
- Multivariate data analysis (including unsupervised and supervised approaches)
- The importance of statistical validation of results
- Computational approaches for metabolite identification and translation of results into biological knowledge
- What are the future challenges for data processing and analysis in metabolomics

Course link: https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/Metabolomics-Data-Processing-and-Data-Analysis.aspx

25 Oct 2019

Introduction to Metabolomics for the Clinical Scientist

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

Overview
This one-day course in partnership with the Phenome Centre Birmingham provides clinicians with an overview of the metabolomics pipeline highlighting the benefits of this technique to the medical field and an introduction to the Phenome Centre Birmingham and the MRC-NIHR National Phenome Centre.
The course provides a suitable introduction to metabolomics prior to taking additional training courses at either the Birmingham Metabolomics Training Centre or the Imperial International Phenome Training Centre.

Metabolomics Events

Topics Covered

- Introduction to the Phenome Centre Birmingham and the Imperial MRC-NIHR National Phenome Centre showcasing facilities and expertise available.
- Introduction to metabolomics
- Importance of experimental design and sample collection
- Overview of technologies available for data acquisition highlighting discovery phase profiling technologies and targeted platforms for the validation of biomarkers
- Overview of technologies available for data analysis
- Case studies – large-scale metabolic phenotyping, translation to targeted assays, clinical practice
- Question and answer session with the experts

Course link:
https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/introduction-metabolomics.aspx

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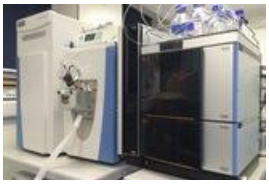
BIRMINGHAM METABOLOMICS TRAINING CENTRE

6-8 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/q-exactive.aspx

Metabolomics Events

BIRMINGHAM METABOLOMICS TRAINING CENTRE

20-21 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.

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 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
Postdoctoral Researcher in the functional metabolic profiling of lipid mediators in lung disease	Karolinska Institutet	Solna, Sweden	26-Apr-19	26-May-19	Nature Careers
Postdoctoral Researcher in the molecular profiling of urinary markers of lung disease	Karolinska Institutet	Solna, Sweden	25-Apr-19	24-May-19	Nature Careers
Various Positions	Lab and Research Manager: Mass-Spectrometry		23-Apr-19		Metabolomics Association of North America Jobs
Lab and Research Manager: Mass-Spectrometry	Icahn School of Medicine at Mount Sinai	New York, New York, USA	12-Apr-19	Until filled	Metabolomics Society Jobs
Metabolomics Specialist	Friedrich Schiller University Jena	Jena, Germany	3-Apr-19		Friedrich Schiller University Jena
Postdoctoral Fellow in Metabolomics and Lipidomics -	University of Washington	Seattle, Washington, USA	3-Apr-19	Until filled	Metabolomics Society Jobs
Postdoctoral Researcher in the molecular profiling of urinary markers of lung disease	Karolinska Institutet	Stockholm, Sweden	1-Apr-19	30-Jun-19	Metabolomics Society Jobs
Postdoctoral Researcher in the functional metabolic profiling of lipid mediators in lung disease	Karolinska Institutet	Stockholm, Sweden	1-Apr-19	30-Jun-19	Metabolomics Society Jobs
Assistant/Associate Professor in Metabolomics of Adaptive Responses	University of California, Riverside	Riverside, California, USA	27-Mar-19	Until filled	Metabolomics Society Jobs
Postdoctoral Researcher in Computational Metabolomics	Institute for Biomedicine, Eurac Research	Bolzano, Italy	11-Mar-19	Until filled	Eurac Research
Lipidomics/ Metabolomics Associate Specialist or Specialist	University of California, Riverside	Riverside, California, USA	03-Mar-19		University of California, Riverside
Postdoctoral Position in Cheminformatics	The Metabolomics Innovation Centre	Edmonton, Alberta, Canada	19-Feb-19	Until filled	University of Alberta

Jobs Offered (continued)

Job Title	Employer	Location	Posted	Closes	Source
Staff Associate/Senior Staff Associate-LCMS Biomarkers Core Laboratory	Columbia University	New York, NY, USA	04-Feb-19	Until filled	Metabolomics Society
Associate Researcher Position in Mass Spectrometry and Exposomics	Icahn School of Medicine at Mount Sinai	New York, New York, USA	23-Jan-19	Until filled	Icahn School of Medicine at Mount Sinai
Postdoctoral Fellow in Mass Spectrometry and Exposomics	Icahn School of Medicine at Mount Sinai	New York, New York, USA	23-Jan-19	Until filled	Icahn School of Medicine at Mount Sinai

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.

- **There are currently no listings**