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Metabolomics Society News

Conference Corner

Registration and Abstract Submission for Metabolomics 2019 is open!

The 15th Annual Conference of the Metabolomics Society will be in The Hague, The Netherlands from June 23-27, 2019, in the World Forum conference centre in The Hague. This jubilee edition is expected to draw a record number of participants, making it the largest Society meeting to date. On June 23-24, 2019, we will see a new high of 18 pre-conference workshops, offering an ideal learning opportunity for early-career scientists.

New elements to the programme are an additional six Introduction to the Field sessions where leading PIs give an overview of their field in small-scale interactive sessions and Career Night on Sunday June 23. At Career Night, employers from academia and industry are posting their job openings, giving the opportunity to early-career and more experienced researchers looking for a next step in their career to meet in person in an informal setting. Several career-related workshops will be taking place during this time.

The conference itself will focus on the applications of metabolomics in academia and industry. The plenary keynote lectures will be given by researchers, not necessarily performing metabolomics analyses themselves, but rather they use and integrate metabolomics in their lines of research. We especially encourage early-career researchers to participate in Metabolomics 2019, and therefore we expect a record number of travel grants will be available, as well as a conference mobile app.

Visit us online at <http://www.metabolomics2019.org/>. The website will be continuously updated, with the latest confirmed speakers and workshops. We would like to welcome you all to The Hague in June 2019. And last but not least: the complimentary conference dinner will be at a Beach Club!



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



Jules Griffin
Metabolomics Society
President

Board of Directors

Words From the President

This month's Board Meeting we have discovered that we might be a victim of our own success – or at least the success of the field!

The Society has provided sponsorship for small-scale metabolomics meetings across the globe for several years. We run two schemes – one aimed at our affiliate networks and another aimed directly at members that are putting on meetings. We've had several members contact us for conference support and so Horst Schirra has been revamping the scheme. He has come up with a system where applications will be judged on a trimester basis depending on when the conference is. So, if your meeting is in June-September of this year you need to send your application in by the end of March, if the meeting is October-January then the application needs to be in by the end of July and if its February-May then the application needs to come in by the end of November in the previous year. What this will allow us to do is to judge a field of applications and make sure the funding goes to the most deserving cases. If you are thinking of putting on a meeting, I encourage you to take a look at the Society webpage and make sure you get your application in early!

Jules Griffin

Members Corner

Early-Career Members Network (EMN)

The 2019 EMN Webinar Series has Started!

Our first EMN webinar in this year's series was held on March 1, 2019 (15:00-16:00 Eastern Time (US)). Dr. Ping-Ching Hsu (Department of Environmental and Occupational Health at the University of Arkansas for Medical Sciences (UAMS)) discussed her perspectives, innovative skills, first-hand experiences, and novel findings in using metabolomics as major approach to study tobacco toxicology. Here is more information of her laboratory:

<https://cancer.uams.edu/2018/10/ping-ching-hsu-ph-d/>

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

Next, we're going to hear from Dr. Pierre-Hugues Stefanuto (University of Liège, Organic Biological Analytical Chemistry Group) about the Multidimensional Chromatography Workshop held in January this year. He is going to give us an overview on complementarity between chromatography and MS for non-targeted analysis, chemical validation and compounds ID, and how to publish this information. The date and time for the Webinar will be published soon.



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@metabolomicsociety.org

Membership Enquiries

membership@metabolomicsociety.org

EMN Bursary Program 2019

The application deadline was February 28, 2019. Winners will be announced in April on the Metabolomics Society website. Selected abstracts and conference reports will be published in MetaboNews and on the Metabolomics Society website.

New to metabolomics or stuck with a problem? We recommend the Metabolomics wiki and Metabolomics Forum. Follow us on Twitter ([@MetabolomicsSoc](https://twitter.com/MetabolomicsSoc)) and Facebook ([EMN.metabolomicssociety](https://www.facebook.com/EMN.metabolomicssociety)) to stay up-to-date on all news and upcoming events.

Other News

Honorary Fellows of the Metabolomics Society

An Honorary Fellowship is a significant lifetime award granted by the Metabolomics Society to exceptional members of our community. Commissioned in 2012, and with up to two awards each year, the Board of Directors welcomes nominations from Members for 2019 Fellowships, with a **closing date of March 30, 2019**.

See <http://metabolomicsociety.org/awards/honorary-fellowships> for further details about the two categories of awards. Each nominee can be nominated for only one of the categories. The Board will consider only complete nomination packages, and these consist of the five items mentioned on the web page.

Metabolomics Society Career Medals

We are excited to announce new Society awards which seek to recognize the outstanding contributions of individuals to the field of metabolomics through the presentation of up to two Metabolomics Society Medals.

These awards are open to all Society members who meet the eligibility criteria. While research contributions are of primary importance, other contributions, including the teaching of metabolomics and/or service to the field or the society will also be strongly considered. There will be up to two medals awarded each year in the following categories:

- The Metabolomics Society Medal is for mid-career members of the society and is open to those members who have been awarded a PhD 10-15 years prior to the closing date for nominations in each round. In 2019, this means your PhD must have been awarded **between 2004 and 2009**.
- The President's Award recognizes outstanding achievements in metabolomics by younger members of the Society or society members. It is available for Society members who have been awarded a PhD no more than 5-10 years prior to the closing date prior to the closing date for nominations in each round. In 2019, this means your PhD must have been awarded **between 2009 and 2014**.

See <http://metabolomicsociety.org/awards/metabolomics-society-career-medals> for further details about the new awards.

The application closing date is **March 30, 2019**.



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www.chenomx.com

Click to view a 2018 publication list.

SpOtlight



Object Oriented Data Analysis (OODA)

Finding untargeted metabolomics peak intensity differences..

This Spotlight article introduces new software for statistical analysis of LC/MS untargeted metabolomics data which has features that distinguish it from current software.

- First, our software is automatic, unbiased, and fast (runs in a few hours) identifying all RT x m/z locations where intensity levels between two groups are statistically different.
- Second, our software has increased power to detect differences by analyzing the raw, unmanipulated (e.g., netCDF, mzXML) data.
- Third, our software uses a single statistical test avoiding problems of analyzing only things that look different and multiple testing.

How does a statistician see untargeted metabolomics data?

Untargeted metabolomics data is a surface where the intensity height at RT x m/z locations represent the number of molecules of possible interest in a sample (see [Figure 1](#)). A researcher would be interested in the intensity bumps, and if they are of different heights in different samples. Problems arise from turning this surface into a few hundred numbers indicating peak heights such as bias, multiple testing, and loss of information and power. A statistician would prefer to analyze this data in its natural form as surfaces without all the data reduction.

A solution is **Object Oriented Data Analysis (OODA)** which has been developed during the last 20-30 years using statistical tools to analyze complex data such as surfaces like [Figure 1](#).

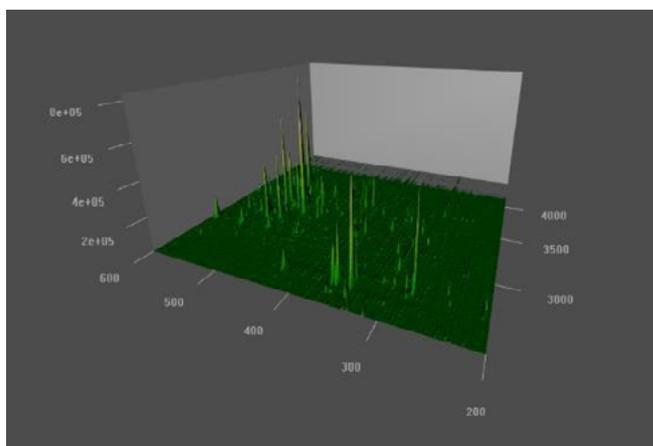


Figure 1
RT x m/z x Intensity surface for a sample from the xcms faahKO data

How does OODA analyze untargeted metabolomics data?

BioRankings' software uses advanced OODA statistical methods we and others have developed. To illustrate, we use xcms faahKO data and focus on m/z from 327.1 – 327.2 and RT from 3350 – 3550 shown in **Figure 2** left column. The top plot shows the intensity values for the KO mice (black lines) and wild type mice (red lines) at each RT. A permutation test was done (bottom plot) with the dashed blue line at P = 0.05. Where the red line goes above the blue line the two groups are statistically different – roughly between RT 3420 – 3430. This was done with no preprocessing, as a single test, and retaining all information.

The test can be applied to any range of m/z and RT values. The right column of **Figure 2** shows a wider m/z and RT range with 4 significant peak differences, including the first difference above RT = 3400, and, interestingly, a small peak just below RT = 3300 that probably would have been missed with other methods. Again, this was done with no preprocessing, as a single test, and retaining all information.

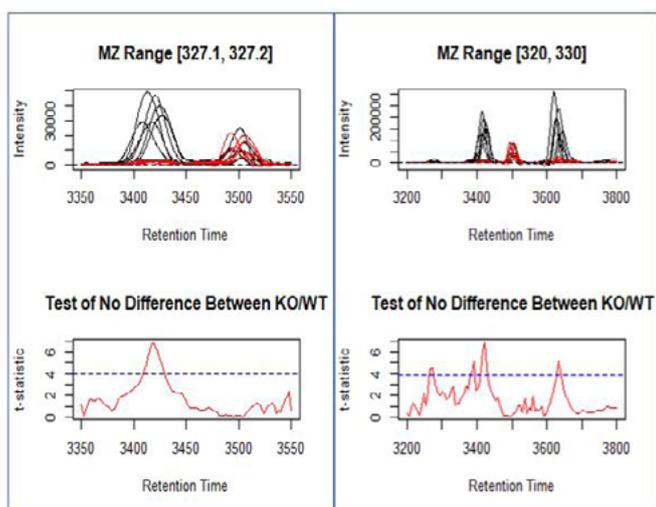


Figure 2
OODA of xcms faahKO data showing statistical differences between two groups of mice

What else can OODA do?

OODA provides a wide range of methods for complex data. Variability of peaks is analyzed by **OODA PCA** (see **Figure 3**). The lower plots show 66.7% of the variability has to do with intensity level (height) and 22.2% with shift along the RT axis. The solid line is the mean of the curves, and the '+++'/'---' lines the range of variability.

Other methods include **OODA mixture models** to disentangle mixture of isomers, and **OODA regression** to measure how covariates impact metabolomic surfaces.

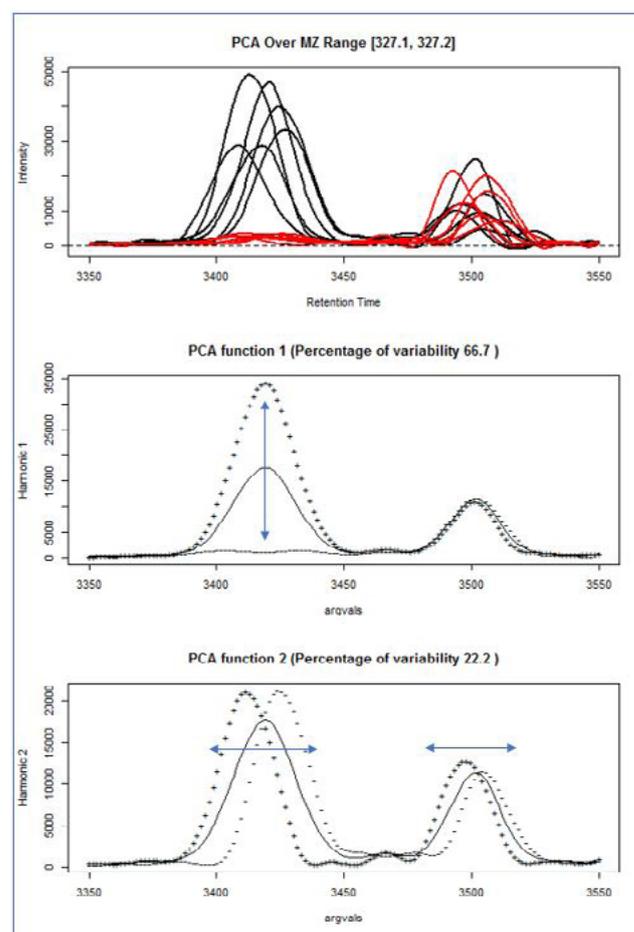


Figure 3
OODA PCA allows intensity surfaces to be decomposed into sources of variability

*Why a statistician should be concerned
about current approaches for finding peak
differences in metabolomics data?*

Turning metabolomics data into a set of single number peak heights is like telling the hiker that Mount Everest is 20,030 feet high but nothing about the area around it or how to climb it. What needs to be done is for new statistical methods to be developed for this new data to avoid the following statistical errors:

- 1.** HARKing: Finding and testing peaks that look different is called Hypothesizing After Results Known and produces the wrong results. Hypothesis tests are only correct if applied before looking at the data – P values from HARKing are not valid.
- 2.** A lot of testing: Doing this on hundreds of peaks is a multiple testing problem where P values need to be adjusted. However, because of the complete lack of independence among peaks, and the fact that the ‘calculated P values from HARKing’ are not ‘P values’, there is no framework for how to do this adjustment or interpret the results.
- 3.** Throwing away information: Turning a gigabyte or more of data from a sample into a set of a few hundred numbers, one for each peak, clearly tosses out information about the sample that can be important to the researcher and reduces the power to detect differences.

Try our software for free and let us know your thoughts

We invite you to try our software with your samples from two groups. You will get a fast (a few hours) analysis that identifies all the RT x m/z regions where peak intensities are statistically different between the two groups ($P < 0.05$). All we ask in return is you tell us what you think and what you would like to see in future software.

**If interested in learning more please contact:
Bill Shannon, PhD, MBA, at BioRankings
(bill@biorankings.com; +1-314-704-8725).**

Recent Publications

Recent Publications

Recently published papers in metabolomics

- [Non-invasive differentiation of non-rejection kidney injury from acute rejection in pediatric renal transplant recipients](#)
- [Edible nuts deliver polyphenols and their transformation products to the large intestine: An in vitro fermentation model combining targeted/untargeted metabolomics](#)
- [Gene expression studies and targeted metabolomics reveal disturbed serine, methionine, and tyrosine metabolism in early hypertensive nephrosclerosis](#)
- [Recent advances in the metabolomic study of bladder cancer](#)
- [Circulating anthocyanin metabolites mediate vascular benefits of blueberries: insights from randomized controlled trials, metabolomics, and nutrigenomics](#)
- [Untargeted metabolomics and inflammatory markers profiling in children with Crohn's disease and ulcerative colitis - a preliminary study](#)
- [Targeted metabolomics of whole blood using volumetric absorptive microsampling](#)
- [A combined targeted/untargeted LC-MS/MS-based screening approach for mammalian cell lines treated with ionic liquids: Toxicity correlates with metabolic profile](#)
- [¹H NMR metabolomic analysis of skin and blubber of bottlenose dolphins reveal a functional metabolic dichotomy](#)
- [Breast cancer risk in relation to plasma metabolites among Hispanic and African American women](#)



Metabolomics Events

**BIRMINGHAM
METABOLOMICS**
TRAINING CENTRE



11 Mar 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.

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>

Metabolomics Events

11-13 March 2019

5th Annual Metabolomics Symposium on Clinical and Pharmaceutical Solutions through Analysis (CPSA Metabolomics 2019)

Venue:

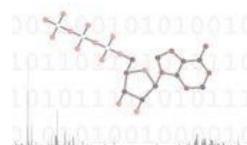
The University of Florida Clinical & Translational Science Institute, Gainesville, Florida USA

Make plans to attend the 5th Annual Metabolomics Symposium on Clinical & Pharmaceutical Solutions through Analysis (CPSA Metabolomics 2019). This unique event is highly interactive and dedicated to the needs of the clinic. The program features updated perspectives and experiences on clinical and pharmaceutical analysis. Imagination and stimulating discussion are central to each CPSA Metabolomics session and event.

Goal

The goal of CPSA Metabolomics is to provide in-depth review of innovative technology and industry practices through open discussion of industry-related issues and needs. This annual event is specifically geared to the needs of professionals attempting to keep pace with faster development times and technology marketing managers attempting to benchmark emerging trends.

For further information, please visit <http://www.cpsa-metabolomics.com/2019/index.shtml>.



18 March - 12 April 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>

Metabolomics Events



1-3 April 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>



4-5 April 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, 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>



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

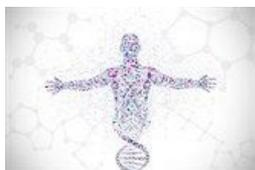
Metabolomics: Understanding Metabolism in the 21st Century

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



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>

9-11 Oct 2019

Introduction to Metabolomics for the Microbiologist

Venue:

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

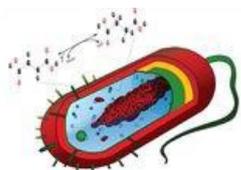
Overview

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>

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



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, 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/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
Various Positions			18-Feb-19		Metabolomics Association of North America
Postdoctoral Position in Cheminformatics	The Metabolomics Innovation Centre	Edmonton, Alberta, Canada	19-Feb-19	Until filled	University of Alberta
Metabolomics Core Manager	UC Davis	Davis, California, USA	19-Feb-19	15-Mar-19	Metabolomics Society
Metabolomics Scientist, Phytochemistry	Plant & Food Research	Palmerston North, New Zealand	7-Feb-19		Science New Zealand
Staff Associate/Senior Staff Associate-LCMS Biomarkers Core Laboratory	Columbia University	New York, NY, USA	4-Feb-19	Until filled	Metabolomics Society
Post-doctoral fellowship, Comprehensive Cancer Center	Ohio State University	Columbus, Ohio, USA	18-Jan-19	15-Mar-19	Metabolomics Society
Tier 2 Canada Research Chair in Biomedical Metabolomics	Queen's University	Kingston, Ontario, Canada	20-Dec-18	Until filled	Metabolomics Society
Ph.D. Position on Mass Spectrometry-Based Analysis of Drug Metabolites	University of Basel	Basel, Switzerland	26-Dec-18	Until filled	Metabolomics Society
Analytic-Specialist in Cell Culture Research (M/F)	Roche	Penzberg, Bavaria, Germany	9-Jan-19	Until filled	Metabolomics Society
Postdoctoral Fellow in Mass Spectrometry and Exposomics	Icahn School of Medicine at Mount Sinai	New York City, NY USA	31-Jan-2019	Spring 2019	Metabolomics Association of North America
Postdoctoral Fellow in Epigenetics and Metabolism	Van Andel Research Institute	Grand Rapids, Michigan, USA	22-Feb-19		Van Andel Research Institute
Associate Researcher Position in Mass Spectrometry and Exposomics	Icahn School of Medicine at Mount Sinai	New York City, NY USA	31-Jan-2019	Spring 2019	Metabolomics Association of North America

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**
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