# MetaboNews

MARCH 2019 Vol 9 Issue 3

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

# Metabolomics Society News

### Conference Corner

From June 23-27, Metabolomics 2019 will take place in The Hague, The Netherlands. It promises to be one of the largest Metabolomics conferences to date, a conference you really will not like to miss. The programme of the conference is shaping quickly; all plenary keynote lectures, most of the pre-conference workshops and half of the session keynotes are now confirmed. Currently we welcome abstracts for oral presentations and posters; the deadline for oral presentations is March 31 and for posters April 26.

The early bird deadline for registration closes on March 31. It offers very significant savings in comparison to later registrations; so, register NOW!

Visit the website <u>www.metabolomics2019.org</u>



### Members Corner

#### Early-Career Members Network (EMN)

#### The EMN Webinar Series 2019: Coming Up!

It is our great pleasure to welcome Dr Hiroshi Tsugawa from RIKEN institute, Japan as the 3rd webinar series' speaker this year. The EMN webinar will be held on April 23rd (3pm PST, 5pm CST, 6pm EST, 11pm GMT), 24th (12am CET, 7am China Time, 8am Japan Time, 10 am AEDT), 2019 under a topic of **Computational mass spectrometry in metabolomics to deepen the understanding of metabolism.** 

He will introduce three metabolomics software programs including (1) MS-DIAL for untargeted metabolomics, (2) MS-FINDER for structure elucidations of unknowns, and (3) MRMPROBS for targeted metabolomics. These programs are demonstrated to perform the comprehensive analyses of primary metabolites, lipids, and plant specialized metabolites where unknown metabolites are also untangled with various methodologies including stable isotope labeled organisms, metabolite class recommendations, and integrated metabolome network analyses. In addition, a computational workflow to link untargeted and targeted metabolomics will also be highlighted in this talk.



#### Metabolomics Society News | Members' Corner & Other News



METABOLOMICS SOCIETY EARLY- CAREER MEMBERS NETWORK

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

#### **General Enquiries**

info@metabolomicssociety.org

Find out his expertise at the RIKEN PRIMe website (<u>http://prime.psc.riken.jp/</u>)

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

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

### Membership News

Thank you for your continued support of the Metabolomics Society. We encourage you to renew your membership online now if you have not already done so. By renewing now, you will continue to enjoy our range of member benefits. To renew your membership, simply log into your account <u>here</u>.

#### Member benefits include:

- 1. Networking and information exchange with an international membership of professionals devoted to furthering metabolomics related science: via conferences and workshops, the Society's many Interest Groups, and social media including the Society's Facebook page and Twitter feed
- 2. Discounted registration fees for Metabolomics Society conferences
- **3.** Receive information and electronic notices of metabolomics conferences, workshops and seminars
- 4. Posting of job adverts on the Society's website
- 5. Apply for funding for small metabolomics events and meetings
- **6.** Online access to conference and workshop presentation videos, including exclusive Members Only content
- 7. Access to research and training webinars on metabolomics science
- 8. Apply for Student Travel Awards
- 9. Apply for Early Career Researcher Travel Awards
- 10. Eligible to vote in Society elections and to stand for Office\*\* within the Society

\*\*Not applicable for Student Members

#### Other News

#### Call for Nominations 2019 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 these Fellowships.

See <u>http://metabolomicssociety.org/awards/honorary-fellowships</u> 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 News | Members' Corner & Other News

#### **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 to 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 <u>http://metabolomicssociety.org/awards/metabolomics-</u> <u>society-career-medals</u> for further details about the new awards.







# Dr. Robert Hall

**Professor of Plant Metabolomics Deputy Business Unit Manager** Wageningen University & Wageningen Plant Research The Netherlands

# Short Biography

Professor Dr. Robert D Hall gained a PhD in plant biotechnology and enzymology (Edinburgh, 1984) and has subsequently completed about 35 years research experience, including 25 years project/group management experience.

He moved to The Netherlands in 1987 where he currently works at Wageningen Plant Research as Deputy Business Unit Manager Bioscience (www.pri.wur.nl/uk/). He also holds a Special Professorship in Plant Metabolomics at Wageningen University. He is co-founder of the Netherlands Metabolomics Centre (www. metabolomicscentre.nl) and currently serves as Chair of the Supervisory Board.

He(co)organised the first ever international metabolomics conference in Wageningen in 2002, the international Metabolomics Society conference in Amsterdam in 2010 and is Co-Organiser of the Society's 2019 meeting in The Hague. He was on the Board of the international Metabolomics Society from 2008-2014 and was the elected President (2010-2012). He was awarded an Honorary Lifetime Fellowship of the Society in 2015. He is scientific advisor/member of a number of (inter)national research committees coordinating research strategy and funding both in Europe and North America.

His primary research activities are now centred on functional genomics and developing metabolomics technologies for application in plants for both science and industry (www.metabolomics.nl). He is on the Editorial Boards of Frontiers in Metabolomics, and the journal Metabolomics. He has completed nearly 200 publications of which 75% are in peer-reviewed journals and he has edited three books including two on Plant metabolomics.



# Interview Q&A



Most crop plants are basically chemical factories producing for example, the nutrients we need to survive daily, but plants are also sources of perfumes, insecticides, toxins, pharmaceuticals, etc. Plants are also the cleverest organic chemists on the planet. It is therefore not surprising that we, as a plant science organisation, recognised early how metabolomics might move us forward in our understanding of plant metabolism. One of the first initiatives we took was to get the community together by organising, together with Raoul Bino, the first ever metabolomics conference in Wageningen in 2002. Out of this came the Plant Metabolomics Forum which in 2005 was merged into the international Metabolomics Society.



Since 2001 our group within Wageningen Plant Research has focused on applying our research efforts to the value of both industry and society but we try to do this based on a firm foundation of fundamental research. The plant breeding and food industries are regularly faced with complex questions related to food quality, disease resistance, flavour and fragrance, etc. These are often issues not directly linked to just a single plant compound but rather, to a complex interaction of molecules. Furthermore, the highly sophisticated biochemical potential of plants means our knowledge is often limited in helping us decide where we should look. Untargeted metabolomics is therefore an excellent entry point to help us assess which group of molecules we can best focus on.

# What are some of the most exciting aspects of your work in metabolomics?

I have always wanted to do research which has the potential to have impact on society. Even during my PhD, I insisted that I should work on a topic that could deliver potentially valuable products – in that case foodgrade plant pigments. So, the biggest drive behind my interests and work even today, still relates to our ability to combine research (which, by definition, means exploring the unknown) and a clear end goal - a process or product which has broad applicability be it related to, e.g., food safety, food quality, varietal development, nutritional value, consumer preference, etc. Metabolomics is still a relatively new field with its own significant challenges, and it has been hugely stimulating and rewarding to have been involved in helping get the technology established. The very early establishment of the Metabolomics Society has been instrumental in the overall success of metabolomics as a new technology; the community was both organised and galvanised right at the time the technology was just taking off.

#### What key metabolomics initiatives are you pursuing at your research centre

We run a core facility based on Mass Spectrometry instrumentation and as such we are involved in very diverse projects with often highly-contrasting biological goals. But next to this we have our own specific core research theme which is centred on food production and quality and especially, flavour and fragrance. See the links with the pictures:



Metabolomics, is a generic technology, applicable to essentially any biological system and we can effectively use this approach to tackle diverse biological questions such as what determines the flavour profile of our food – both fresh materials and after processing; what are the bioactive chemicals in plants which protect them against insect attack; how do plants modify their metabolism as a result of abiotic stress, etc? Recently we have been also testing out GC-Olfactory and cell-based detection methods where we use human receptors as a second (or third) detector! It is then interesting to see how, despite all the technological advances, that e.g. our nose is still in many instances more sensitive than the MS in helping us to detect phenotypically-important compounds not visible in the chromatogram!



Source: Henquet et al. (2016)

# What is happening in your country in terms of metabolomics?

For many years the Netherlands Metabolomics Centre was the centrepoint for the development of metabolomics technologies. While the central funding stopped some time back, we have maintained the NMC as a focal point for new initiatives and we are again establishing a set of local workshops and meetings – also together with our Belgian neighbours. We also have good contacts with industry which helps keep us in touch with the final relevance of what we are doing. Different industrial partners in the plant and food sectors are already exploiting metabolomics in their R&D business.



# MN How do you see your work in metabolomics being applied today or in the future?

As stated above, nearly all our research, including the more fundamental aspects, always has a long(er) term goal of being applied in the context of industrial strategy. This relates both to the technology development aspects – where we aim to deliver analytical procedures to investigate and evaluate biochemical profiles – as well as the technology application aspects where we can deliver biologically-relevant chemical information related to phenotype. Metabolomics approaches are already being exploited within both the breeding and food processing industries.

### As you see it, what are metabolomics' greatest strengths?

Key strengths are of course the scalability of the technology which has truly become high throughput where it is feasible to take on hundreds and indeed thousands of samples. In our case working on plants, the option for an untargeted approach is also a strength when our initial knowledge is limited. We are often faced with hugely complex chemistries which are influenced not only by genetic and environmental factors but also have huge temporal and spatial heterogeneity within the plant organ itself.

# What do you see as the greatest barriers for metabolomics?

I prefer to see it more as a challenge than a barrier but, especially for people working in plant research, our ability to identify robustly and efficiently the metabolites which we can now detect remains a limitation. We often say we don't always actually need to know what a molecule is in order to exploit it – if an "unknown" is statistically-linked to a particular trait we can still use it as a marker for that trait. However, as biologists we of course will much better understand the system as a whole and the mechanisms behind a trait when we can link a metabolite first to a specific pathway and then importantly, to the genes behind its production - be these structural genes or transcription factors controlling gene expression. I see this aspect as being the biggest challenge facing us for the next 5 – 10 years.

#### What improvements, technological or otherwise, need to take place for metabolomics to really take off?

I would say that metabolomics has certainly already taken off quite considerably, but we are not yet at our destination. Aspects of standardisation, metabolite identification, quantification and data analysis and visualisation remain tasks requiring additional attention. We are still not there yet with true standardisation of many methodologies for data generation and efficient data storage and mining of our ever-growing databases are continuing challenges.



# How does the future look in terms of funding for metabolomics?

Funding is forever an issue. Average success rates for EU projects are now below 10% and for certain national funding sources rates can also approach this level. This is hugely inefficient and a major waste of effort and a massive cause of frustration. In the Netherlands a major part of scientific funding is also linked to industry and requires their (financial) support. As an applied scientist this is not at all a bad idea, but I feel we have lost the balance and many companies have become saturated with projects such that they are stepping out of certain calls. This does not make our lives any easier!

### What role can metabolomics standards play?

Related to the points mentioned above, the use of chemical standards to both allow full quantification as well as metabolite identification (MSI level 1) is essential for future developments and success of the technology. Standard methodologies as well as standardised data repository resources are not simple but are nevertheless hugely important for long – term value. Thankfully, the community is now united in several working groups to help coordinate and tackle these challenges.

# Do you have any other comments that you wish to share about metabolomics?

Of course I cannot miss this opportunity to advertise the next official meeting of the international <u>Metabolomics</u> <u>Society</u> which we are organising in The Hague next year! The last time we organised this meeting was in 2010 in Amsterdam which was a huge success. For 2019 we cannot guarantee the weather we had then (or the excitement of the concurrent World Cup finals) but we do aim to make this the biggest and best metabolomics meeting ever! We will have for the first time four parallel sessions, lots of workshops in the days before the meeting, a conference dinner on the beach, etc. Every self-respecting metabolomicist would be mad to miss it!



#### Follow the plans on www.metabolomics2019.org!



# **Recent Publications**

Recently published papers in metabolomics

- <u>A Metabolomic Study of the Variability of the Chemical Composition of Commonly</u> <u>Consumed Coffee Brews</u>
- The association of sleep with metabolic pathways and metabolites: evidence from the Dietary Approaches to Stop Hypertension (DASH)-sodium feeding study.
- An untargeted metabolomic strategy based on liquid chromatography-mass spectrometry to study high glucose-induced changes in HK-2 cells.
- <u>Metabolome-based signature of disease pathology in MS.</u>
- Mitochondria in precision medicine; linking bioenergetics and metabolomics in <u>platelets.</u>
- <u>Recent developments in metabolomics-based research in understanding transgenic</u> <u>grass metabolism.</u>
- Resolving coral photoacclimation dynamics through coupled photophysiological and metabolomic profiling.
- Impaired clearance of sunitinib leads to metabolic disorders and hepatotoxicity.
- Identification and characterization of metabolite quantitative trait loci in tomato leaves and comparison with those reported for fruits and seeds.
- <u>De novo structure determination of 3-((3-aminopropyl)amino)-4-hydroxybenzoic</u> <u>acid, a novel and abundant metabolite in Acinetobacter baylyi ADP1.</u>
- <u>Metabolomics of Dynamic Changes in Insulin Resistance Before and After Exercise</u> in PCOS.

#### BIRMINGHAM METABOLOMICS TRAINING CENTRE





#### 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

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

- Data analysis, detecting outliers and drift, and pretreatment 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



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.

#### **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: <u>https://www.canmetcon.ca/program</u>
- Registration: <u>https://www.canmetcon.ca/registration</u>
- Abstract Submission: <u>https://www.canmetcon.ca/abstract-submission</u>



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



# 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:

13 May - 7 June 2019

- 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 <u>http://www.rsc.org/events/detail/29574/</u> challenges-in-analysis-of-complex-natural-mixtures-faraday-discussion

#### BIRMINGHAM METABOLOMICS TRAINING CENTRE



#### 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:

 $\underline{https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/Metabolomics-MOOC.aspx}$ 

# 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: <a href="http://biomic.web.auth.gr/workshop2019/">http://biomic.web.auth.gr/workshop2019/</a>







### 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



#### BIRMINGHAM METABOLOMICS TRAINING CENTRE



# 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

#### BIRMINGHAM METABOLOMICS

# 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.



#### **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:** <u>https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/introduction-metabolomics-microbiologist.aspx</u>



#### BIRMINGHAM METABOLOMICS TRAINING CENTRE



# 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 sn

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- Processing direct infusion mass spectrometry data
   Processing liquid chromatography-mass
- spectrometry data
- Reporting standards and data repositories

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

- Data analysis, detecting outliers and drift, and pretreatment 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

#### BIRMINGHAM METABOLOMICS TRAINING CENTRE



#### 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

#### 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



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

# 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 Fellowship, Food Research Center	University of São Paulo	São Paulo, Brazil	20-Mar-19	25-Apr-19	<u>University of São</u> <u>Paulo</u>
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	3-Mar-19		<u>University of</u> <u>California,</u> <u>Riverside</u>
Post-Doctoral Scholar - Metabolomics/ Proteomics		Lexington, KY, USA	26-Feb-19	22-Apr-19	<u>University of</u> <u>Kentucky</u>
Postdoctoral Position in Cheminformatics	The Metabolomics Innovation Centre	Edmonton, Alberta, Canada	19-Feb-19	Until filled	<u>University of</u> <u>Alberta</u>
Various Positions			18-Feb-19		<u>Metabolomics</u> <u>Association of</u> <u>North America</u> <u>Jobs</u>
Metabolomics Scientist, Phytochemistry	Plant & Food Research	Palmerston North, New Zealand	7-Feb-19		<u>Science New</u> Zealand
Staff Associate/Senior Staff Associate-LCMS Biomarkers Core Laboratory	Columbia University	New York, NY, USA	4-Feb-19	Until filled	<u>Metabolomics</u> <u>Society</u>
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	<u>Icahn School</u> of Medicine at <u>Mount Sinai</u>
Postdoctoral Fellow in Mass Spectrometry and Exposomics	Icahn School of Medicine at Mount Sinai	New York, New York, USA	23-Jan-19	Until filled	<u>Icahn School</u> of Medicine at <u>Mount Sinai</u>
Analytic-Specialist in Cell Culture Research (M/F)	Roche	Penzberg, Bavaria, Germany	9-Jan-19	Until filled	<u>Metabolomics</u> <u>Society</u>
Ph.D. Position on Mass Spectrometry- Based Analysis of Drug Metabolites	University of Basel	Basel, Switzerland	26-Dec-18	Until filled	<u>Metabolomics</u> <u>Society</u>
Tier 2 Canada Research Chair in Biomedical Metabolomics	Queen's University	Kingston, Ontario, Canada	20-Dec-19	Until filled	<u>Metabolomics</u> <u>Society</u>



#### 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 (<u>metabolomics.innovation@gmail.com</u>). Upon review, a limited number of job submissions will be selected for publication in the Jobs Wanted section.

#### • There are currently no listings