MetaboNews

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

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

Metabolomics Society News

Conference Corner

Important Note from the Society BOD as of 4th March 2020

Dear Colleagues,

As you will all be aware the recent Coronavirus outbreak in Wuhan, China has now spread to many countries across the globe. The Metabolomics Society Board of Directors and the Local Organizing Committee of the Shanghai meeting have been monitoring the situation closely. Because of the current status of the outbreak and the travel restrictions in place we have taken the decision to re-schedule the conference. We want to convey to the membership that this has been forced upon us by the magnitude of the global crisis and apologize for moving the dates of this meeting. We are currently renegotiating dates with the conference center and expect the meeting will be held Dec 7-11, 2020. Registration, abstract submission, and workshop deadlines will all be adjusted accordingly. New dates will be formalized, and email announcements sent ASAP. As you will be aware, we find ourselves in quite exceptional circumstances and we thank you for your patience.

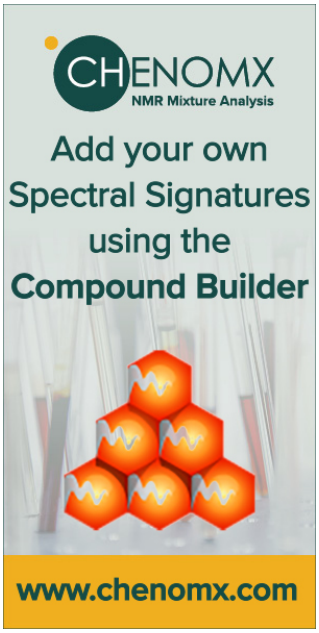
The board of the Society is in close and regular contact with the Local Organizing Committee of the 2020 Metabolomics Society Conference in Shanghai. We are monitoring the situation on the ground, are discussing recent events, and will be sending along more information in the coming weeks when we have updates.

Our thoughts are with those affected in China and globally. We hope the virus outbreak will come to a swift end. If you have any questions or comments, the Metabolomics Society welcomes any feedback and will respond to your inquiries. Further information can be found on the website in the coming weeks as we post updates.

Sincerely,

Board of Directors
Metabolomics Society

Jules Griffin
Metabolomics Society President



Board of Directors

Words From the President

As you will see from the official statement made by the Board of Directors of the Society this has been a tough month. We have watched as the coronavirus outbreak has spread across the globe and the first thoughts of the Board have been with those affected by COVID-19. We have held a number of emergency meetings to discuss whether the international meeting in Shanghai should go ahead. This has included the Local and International Organising Committees to assess the situation in China and internationally in terms of the outbreak and travel restrictions, the industrial task group to assess travel restrictions in industry and the conference chairs, Jiang Zhu and Huiru Tang to assess the situation in Shanghai. We are faced with a situation where nearly all academic and industry establishments have travel restrictions in place and uncertainty about when the situation will improve. We also want to put the safety of our members at the forefront of any decision. As a result, we have taken the very difficult decision to postpone the meeting from July. We are currently renegotiating with the conference centre and hope to have a date confirmed in December. This decision has not been taken lightly and I would like to thank everyone who has taken part in these difficult discussions. The board is looking into ways we might still meet in June/July virtually so please watch this space for further information. We do hope you will still be able to join us in China in December and meanwhile I hope you and your families are safe during this global emergency.

Jules Griffin
President, Metabolomics Society

Members Corner

Early-Career Members Network (EMN)

New Committee Member
The EMN welcomes Marine Letertre, its newest committee member, who will substitute Jun Zhou. The EMN committee thanks Jun for his contribution and wishes him all the best for the future.

Travel Bursary Program
We are delighted to have received numerous outstanding applications for The EMN Travel Bursary Program. Up to 4 travel grants will be awarded to early-career researchers to cover travel, accommodation costs and conference fees up to $500. Awardees will be announced by April 1st, 2020.

EMN Webinars
Stay tuned for announcements sent over email and posted on our social media platforms.

EMN Social Media
Follow the EMN on Facebook and Twitter for updates and special events.

METABOLOMICS SOCIETY

METABOLOMICS SOCIETY
EARLY- CAREER MEMBERS NETWORK

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Task Groups Corner

Metabolite Identification Task Group

The Metabolite ID Task Group of the Metabolomics Society Needs Your Help!

Request for community feedback for revised reporting standards for metabolite annotation and identification

Dear Metabolomics User,

The Metabolite Identification Task Group of the Metabolomics Society have assessed and revised reporting standards for metabolite annotation/identification based on metabolite structure and experimental evidence provided. These have developed from the 2007 original reporting standards published by Sumner and colleagues. The Metabolomics Society and this task group would like to receive feedback on the revised reporting standards from the future users of the reporting standards, you! The reporting standards can be viewed below and in this PDF.

Proposed reporting standards for metabolite annotation and identification in metabolomics (color-blind friendly)

level	atoms	atomic connections	relative stereo-chemistry	chirality	metabolite ID class	metabolite information level
A	✓	✓	✓	✓	• a single, defined enantiomer • or a single, defined achiral metabolite	• known molecular formula • known structure • known stereochemistry if present • known chirality if present • e.g. tartaric acid (2R,3R)-2,3-dihydroxybutanoic acid
B	✓	✓	✓	X	• one of two enantiomers	• known molecular formula • known structure • known relative stereochemistry if present • unknown chirality • e.g. tartaric acid: enantiomer undefined (2R,3R or 2S, 3S)
C	✓	✓	X	X	• one of a number of stereoisomers • e.g. E/Z geometric or cis-/trans- ring isomers	• known molecular formula • known molecular structure • unknown relative stereochemistry • e.g. tartaric acid diastereomer undefined: 2R, 3S, 2R, 3R or 2S, 3S • oleic acid (Z-isomer) or elaidic acid (E-isomer of 9-octadecanoic acid)
D	✓	X	X	X	• one of a number of positional isomers	• known molecular formula • known functional groups • unknown structure • e.g. $C_{18}H_{34}O_2$: 9-octadecanoic acid or 7-octadecanoic acid
E	✓	X	X	X	• one of a number of possible compounds of known molecular formula	• known molecular formula • unknown structure • e.g. C_2H_6O: dimethylether or ethanol
F	X	X	X	X	• specific spectral features defining a structural class	• unknown molecular formula • known structural class
G	X	X	X	X	• specific spectral features	• unknown molecular formula

Feedback can be provided on this simple form: https://forms.gle/jLUQu1apqL3UQu2A7

We look forward to receiving your input and acting on this feedback.

Many thanks in advance,
The Metabolite Identification Task Group of the Metabolomics Society

International Affiliates Corner

Metabolomics South Africa

Visit www.metabolomics-sa.co.za

30-31 March 2020

Second National Metabolomics Symposium – South Africa

Venue: Ubuntu Chambers at the University of Johannesburg, Kingsway Campus, Auckland Park, Gauteng, South Africa

The African Centre for Gene Technologies (ACGT) and Metabolomics South Africa (MSA) will host a two-day Metabolomics Symposium on 30-31March 2020 in Johannesburg, South Africa. This will be the second national metabolomics symposium, which will be an opportunity for principal investigators, postgraduate students and interested parties to share their metabolomics research and applications. Additionally, the event is intended to foster further collaboration amongst metabolomics researchers within South Africa and across Europe by providing a platform for researchers to network and to identify synergies.

Keynote speakers: Dr. Fabien Jourdan, INRA Toulouse, France; Dr. Reza Salek, IARC/WHO, Lyon, France; Dr. Karl Burgess, University of Edinburgh, UK; Dr. Justine Bertrand-Michel, INSERM Toulouse, France; Dr. Fidele Tugizimana, University of Johannesburg/Omnia, RSA; Prof. Carina Mels, North-West University, RSA; Dr. Grace Ijoma, University of South Africa, RSA.

Registration: https://www.surveymonkey.com/r/2020MetabolomicsSymposium
Contact: molati.nonyane@up.ac.za

1-3 April 2020

Advanced Metabolomics Workshop – South Africa

Venue: Bioinformatics Centre, University of Pretoria, Pretoria, South Africa

The African Centre for Gene Technologies (ACGT), in collaboration with MSA, has organized a three-day Advanced Metabolomics Workshop to provide a platform to learn advanced fundamentals, address key issues and challenges in the field of metabolomics. The workshop is designed to include a mixture of lectures, interactive round table discussions and computer-based practical sessions. The workshops will be facilitated by a team of renowned Metabolomics experts, both local and international.

Topics to be covered:

- Metabolomics and other Omics
- Workflows
- Data Mapping
- Data Analysis
- Statistics
- Metabolite Identification
- Standards
- Metabolomics resources
- Lipidomics

Keynote speakers / trainers: Dr. Reza Salek, IARC/WHO, Lyon, France; Dr. Karl Burgess, University of Edinburgh, UK; Dr. Fabien Jourdan, INRA Toulouse, France; Dr. Justine Bertrand-Michel, INSERM Toulouse, France; Dr. Fidele Tugizimana, University of Johannesburg/Omnia, RSA; Dr Aurelia Williams, North-West University, RSA.

Registration: https://www.surveymonkey.com/r/2020AdvancedWorkshop
Contact: molati.nonyane@up.ac.za

Other News

Deadline Extended: Honorary Fellows and Career Medal Nominations

2020 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, with a NEW closing date of June 1, 2020.

See http://metabolomicssociety.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 continue the 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 2020 this means your PhD must have been awarded between 2005 and 2010.

- 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 for nominations in each round. In 2020 this means your PhD must have been awarded between 2010 and 2015.

See http://metabolomicssociety.org/awards/metabolomics-society-career-medals for further details about awards. The NEW application closing date is **June 1, 2020**.

METABOINTERVIEW

Dr. Fabien Jourdan

Senior Researcher
INRAE Toulouse, France
Metabolomics Society Board of Directors

Short Biography

Dr Fabien Jourdan gained a PhD in Computer Science (Montpellier, 2004) and has subsequently completed about 15 years of research experience.

During his PhD and the following year within a software start-up, he studied the structure and visualization of complex networks. This was the exciting early times of social networks and he particularly focused on movie actors' networks, developing algorithms to study their architecture and identify clusters in these large and complex systems. He also developed tools to visualize biological networks and in particular metabolic networks. Then, in 2005, he moved to Toulouse to take a permanent researcher position at INRA to study metabolomics data in the context of metabolic networks. In 2006 he spent one year as a visiting researcher at the Bioinformatics Research Centre of the University of Glasgow where he set up a collaboration with Pr. Mike Barrett and was awarded an ANR-BBSRC grant to pursue his investigations on Trypanosoma brucei parasite metabolism.

After coming back to Toulouse in 2009, with Dr. Ludovic Cottret and Florence Vinson, he set up the MetExplore (www.metexplore.fr) web server for the analysis of omics data in the context of genome scale metabolic networks. Since that date, Fabien Jourdan has been the PI on several national and EU grants with a special focus on the impact of food contaminants on human metabolism. He is now Metabolism and Xenobiotics (MeX) team leader (with Dr. Zalko) at INRAE food toxicology research centre (Toxalim). He is a founding member of France's infrastructure of metabolomics and fluxomics MetaboHub. Finally, he is strongly involved in the activities of the metabolomics community, being on the board of the RFMF (French-speaking Metabolomics and Fluxomics Network) from 2010 to 2015 and serving as President of RFMF from 2015 to 2019. He was elected in 2019 to serve on the Board of Directors of the Metabolomics Society and chaired in 2020 the first European conference in Metabolomics in Toulouse.

Interview Q&A

How did you get involved in metabolomics?

My main interest during my early career was to study the structure of social networks. It may sound far from metabolomics but we recently showed that we can translate social network algorithms to improve metabolic profiling (MetaboRank, Frainay et al. 2019). My move from social networks to metabolomics is following the publication, in the early 2000s, of high impact articles on the topological properties of biological networks including metabolic networks (which have been criticized quite a lot since that date). Following this trend, I was recruited by Dr. Alain Paris as a permanent researcher at INRAE Toulouse in 2005 to develop computational methods to use metabolic networks as a context for the interpretation of metabolomics data. (Figure 1)

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

We develop algorithms and tools (many implemented in the MetExplore web server) to facilitate the interpretation of metabolomics data using metabolic networks. It is really rewarding to be part of the understanding of metabolic modulations in health, toxicology and beyond. It is also quite exciting to translate computational methods from other fields (social networks, recommendation systems) to tackle metabolomics questions. More globally our aim is to identify, based on omics data, modulated sub-networks related to diseases or exposure to chemical compounds. To do so we both use graph-based algorithms and constraint-based modelling. Since our team involves both biologists and computational scientists, we can design experimental setups to obtain the required data for modelling (Figure 2).

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

Our assumption is that metabolic networks will help in better: 1) understanding metabolic modulations, 2) classifying metabolic modes of actions of xenobiotics and diseases, 3) predict intracellular metabolic modulations from extra-cellular/tissular metabolomics, and 4) annotate metabolomics data. These aspects are implemented in several exciting projects we just started. One H2020 EU project, called GOLIATH, aims at developing and validating assays to decipher the effect of Endocrine Disruptors Compounds on metabolism through a combination of techniques starting from cellular models and ending with validation in human cohorts.

I will also coordinate a French-German project on the integration of the various networks which are used in metabolomics: experimental networks (e.g., correlation networks), ontologies and genome scale metabolic networks. All these projects involve a great network of collaborators including leading players from our community like Jules Griffin, Steffen Neumann, Reza Salek, and Michael Witting.

What is happening in your country in terms of metabolomics?

France pioneered the national structuring of metabolomics by the creation in 2005 (one year after the creation of the Metabolomics Society) of the RFMF (French Metabolomics and Fluxomics Network, which was extended in 2015 to French-speaking countries). Thanks to the founders of the RFMF (AM Delort, JC Portais, and D Rolin), the network was built on a great spirit of focusing on including early-career researchers, supporting collective research actions, and organizing a conference each year following a very French mantra "good food, good science" and attended by more than 250 attendees. In January 2020, RFMF and MPF, together with regional and national networks, organized a conference in Toulouse hosting more than 400 attendees. We hope a European-scale event such as this will be pursued in the same spirit with special care taken to include as many EC scientists as possible.
In 2013, France also put a substantial effort in supporting the creation of a national infrastructure in Metabolomics and Fluxomics called MetaboHub. This infrastructure develops new methods and tools which are used beyond MetaboHub (for instance, the galaxy platform Workflow4Metabolomics was endeavored within the consortium). MetaboHub gathers four metabolomics facilities in France (Bordeaux, Clermont-Ferrand, Saclay, and Toulouse) and will soon be officially joined by facilities in western France Corsaire (Nantes and Rennes). MetaboHub was recently awarded a new grant of five years dedicated to the recruitment of staff to develop new analytical and computational methods. Stay tuned, there will soon be several open positions!

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

Metabolomics is now a cornerstone approach in a large range of application fields. It is quite a strong and powerful tool to decipher and understand metabolism. Regarding human health and toxicology, I am convinced that it will be used more and more as part of the decision process (individualized treatments, risk assessment). To achieve this goal, we nevertheless must work on interoperability between techniques, time points, and data. The single cell metabolomics will also help a lot in the future, for instance to better understand cancer heterogeneity. Fluxomics, together with modelling, will allow us to get a more precise and dynamic view of the metabolic activity from cells to individuals. Finally, working on better interoperability with the other omics will allow to more accurately define and understand metabolic systems.

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

Metabolomics' strength resides in its ability to provide data as close as possible to the metabolic phenotype of a cell, a tissue, an organism. Being non-invasive, it is also possible to include the approach in many cohort projects (humans, plants) allowing many breakthroughs in precision medicine for instance. The other strength of metabolomics (which is also sometimes a challenge) is its pluri-disciplinary nature. All the sciences are strongly interconnected and every one of them is enriching the other.
One strength of metabolomics is also its community of researchers. Networking and sharing are key to the success of metabolomics. Perhaps it is the need to emerge within established omics which has drawn the community together. Networks and societies were and are instrumental in that.

What do you see as the greatest barriers for metabolomics?

We, as a community, definitely need to go further in terms of improving FAIRness of metabolomics data. This is crucial if we want to integrate our data and apply predictive models using a large number of datasets. This is of course more challenging than other omics since we use a wide range of analytical tools and set ups, but we need to move in this direction. Especially improving meta-data annotations by using ontologies will be key to reach interoperability.

Concerning networks and metabolomics, there is a need to agree on a shared vocabulary between modelers and scientists producing metabolomics data. For some model organisms, it is currently improving but for many other organisms it is still challenging to accurately map data in genome scale metabolic networks. Hence, we need to improve the dialog between modelers producing genome scale metabolic networks and our community.

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

Metabolomics is already acknowledged in many application fields. We nevertheless need to improve coverage of metabolism for instance by integrating data produced by different analytical platforms. Quantification and flux measures will also improve our understanding of metabolism by providing quantitative and dynamic observations of metabolic modulations.
Regarding genome scale metabolic networks, we need to pursue reconstruction efforts by detailing some metabolic pathways like ones related to lipid metabolism. We also need to find better ways of integrating experimental data in the models, so we improve the prediction accuracy. Metabolism is a highly regulated system, the integration of both metabolic networks and regulatory ones will also be key to improve predictions.

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

There is a growing interest in metabolism (e.g., in cancer) and in metabolites (e.g., natural products). Metabolomics is thus required in many projects to produce data to tackle urgent research questions. To my mind, the big challenge in our field is to find funding for fundamental methodological research which will allow us to unlock current metabolomics limitations (sensitivity, metabolome coverage, data mining). As PIs, we must always fight on two fronts: applied and fundamentals which can be quite challenging and requires a lot of effort.

What role can metabolomics standards play?

As mentioned earlier, FAIR in metabolomics is of upmost importance. Standards are central in this development and it is very important to acknowledge the groups working on this topic (e.g., the Data Standards Task Group within the Metabolomics Society). It is important that the whole community feels involved in this effort and provides feedback so that we reach a well-accepted level of standardization.

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

Research is a collective effort and human aspects are key to reach high level scientific results. That is the reason why we need to include early-career (EC) members in networking activities and scientific projects as soon as possible. It is the path chosen by RFMF for years (namely, RFMF Junior), by the Metabolomics Society (EMN) and other networks. We need to continue our efforts towards ECs. It is really rewarding to see that many of the EC scientists we trained for almost 10 years at the EMBO course coordinated by Reza Salek are now PIs and creating their own groups with very exciting research programs.

I would like to take the opportunity to acknowledge all members of my team for their constant effort, hard work, and great spirit of teamwork as well as all the wonderful scientific mentors I have worked with during my career.

Figure 1. Human metabolic network Recon2.2 visualized in MetExploreViz (*Chazalviel et al. 2018*)

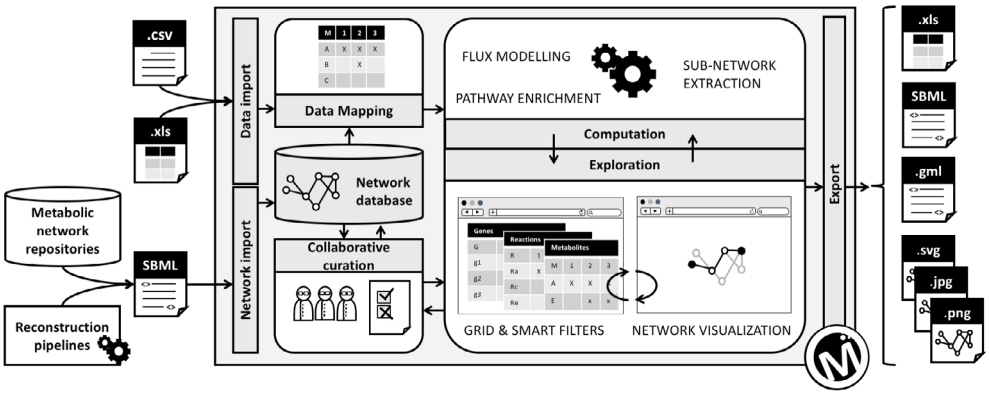

Figure 2. MetExplore overview (*Cottret et al. 2018*)

Recent Publications

Recently published papers in metabolomics

- AlpsNMR: an R package for signal processing of fully untargeted NMR-based metabolomics
- Metabolomic Data Exploration and Analysis with the Human Metabolome Database
- Mass-spec-based urinary metabotyping around parturition identifies screening biomarkers for subclinical mastitis in dairy cows
- Clostridioides difficile Colonization Is Differentially Associated With Gut Microbiome Profiles by Infant Feeding Modality at 3-4 Months of Age
- Aberrant regulation of choline metabolism by mitochondrial electron transport system inhibition in neuroblastoma cells
- Comparing capillary electrophoresis-mass spectrometry fingerprints of urine samples obtained after intake of coffee, tea, or water
- Reversed-phase LC/MS method for polyphosphoinositide analyses: changes in molecular species levels during epidermal growth factor activation in A431 cells
- Evaluating low-intensity unknown signals in quantitative proton NMR mixture analysis
- Metabolic changes in flatfish hepatic tumours revealed by NMR-based metabolomics and metabolic correlation networks
- High Resolution Separations and Improved Ion Production and Transmission in Metabolomics

Metabolomics Events

BIRMINGHAM METABOLOMICS TRAINING CENTRE

30 Mar - 1 Apr 2020

Metabolomics with the Q Exactive

Venue:
Birmingham Metabolomics Training Centre, University of Birmingham, United Kingdom

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

Topics Covered

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

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

30 Mar - 2 Apr 2020

Introduction to Metabolomics Analysis

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

Overview
Application opens: Monday 23 September 2019
Application deadline: Friday 29 November 2019
Participation: Open application with selection
Contact: Meredith Willmott
Registration fee: £650 - Including meals and accommodation

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

BIRMINGHAM METABOLOMICS TRAINING CENTRE

2-3 April 2020

Metabolite identification with the Q Exactive and LTQ Orbitrap

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

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

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

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

21-24 April 2020

Hands-on Data Analysis for Metabolic Profiling

Venue:
Imperial College London, London, United Kingdom

This 4 day course provides a comprehensive overview of data analysis for metabolic profiling studies with data acquired from NMR spectroscopy and Liquid Chromatography-Mass Spectrometry. It combines lectures and tutorial sessions to ensure a thorough understanding of the theory and practical applications.
For more information, click on the link Hands-on Data Analysis for Metabolic Profiling, 21-24 April 2020

BIRMINGHAM METABOLOMICS TRAINING CENTRE

27-29 April & 7-9 Oct 2020

Introduction to Metabolomics for the Microbiologist

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

Overview

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

Topics Covered

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

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

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

27 Apr to 1 May 2020

Hands-On LC-MS for Metabolic Profiling

Venue:
Imperial College London, London, United Kingdom

This week long course aims to cover how to perform a metabolic profiling experiment, from start to finish. It will cover study design, sample preparation, the use of mass spectrometry for global profiling and targeted methodologies and data analysis.

For more information, click on the link Hands On LC-MS for Metabolic Profiling, 27 April – 1 May 2020

30 Apr to 1 May 2020

The Third Annual Canadian Metabolomics Conference

Venue:
Edmonton, Alberta, Canada

The Third Annual Canadian Metabolomics Conference will be held from April 30th - May 1st, 2020 in Edmonton, 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. 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 Edmonton - capital of Alberta.

Conference link:
https://www.canmetcon.ca/

6-10 July 2020

Metabolomics 2020

Venue:
Shanghai, China

Overview

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

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

6-10 July 2020

Introduction to Nutritional Metabolomics

Venue:
Department of Nutrition Exercise and Sports, University of Copenhagen, Denmark

Overview

The course will provide an overview of LC-MS based untargeted metabolomics and its application in nutrition. It will be delivered using a mixture of lectures, hands-on data preparation and analysis, computer-based practical sessions, and discussions. Visits to wet labs and instructions on human sample preparation procedures is included but with minimal hands-on.

The students will go through common steps in a typical metabolomics study using a real-life case. This case study includes collected plasma (or urine) samples from a nutritional intervention. The sample preparation and analysis on UPLC-QTOF has been conducted and the students will further process and analyse the acquired data with various freeware tools (e.g., R, XCMS, MZmine and MetaboAnalyst). They will finally work on identification of relevant metabolites using several web-based structure elucidation tools. The course will conclude by presentations of reports generated by the students based on the case study.

The course will be structured as initial short lectures on theory followed by hands-on exercises, which will teach the students to transfer the theoretical information to practice.

Fee

No fee for the PhD students under the Open Market in Denmark and NOVA partners.
Other participants are to pay a course fee of 300 EUR. Each student must pay and arrange their own travel and accommodation in Copenhagen during the course.

Course link
https://phdcourses.ku.dk/detailkursus.aspx?id=107283&sitepath=NAT

15 July 2020

ISMB 2020 CompMS – Save the date & call for proposals

Venue:
Palais des congrès de Montréal, Montreal, Canada

Overview
Please join us during the ISMB 2020 conference for the Computational Mass Spectrometry (CompMS) COSI session on July 15, 2020 in Montreal, Canada.

The ISMB conference is the world's largest bioinformatics/computational biology conference. Every year it brings together scientists from computer science, molecular biology, mathematics, statistics, and related fields and provides an intense multidisciplinary forum for disseminating the latest developments in bioinformatics/computational biology. The conference fosters fresh dialogues, collaboration and learning opportunities, and is a gathering which shapes the future of the field.

At the heart of the scientific program are ISCB's Communities of Special Interest (COSIs), enabling community involvement and bolstering ISMB's reputation as the leading conference in the field. The CompMS COSI promotes the efficient, high quality analysis of mass spectrometry data through dissemination and training in existing approaches and discussion of new, innovative approaches. The CompMS initiative aims to exploit synergies between different application domains, in particular proteomics and metabolomics.

A strong scientific and technical program showcases the best international developments in bioinformatics and computational biology, making ISMB 2020 a must attend event.

Date: July 15, 2020 (CompMS COSI) / July 12–16, 2020 (ISMB)
Website: https://www.iscb.org/ismb2020

BIRMINGHAM METABOLOMICS TRAINING CENTRE

23-25 Sep 2020

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

Venue:
Birmingham Metabolomics Training Centre, University of Birmingham, United Kingdom

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

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

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

BIRMINGHAM METABOLOMICS TRAINING CENTRE

7-9 Oct 2020

Introduction to Metabolomics for the Microbiologist

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

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

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

Course link

BIRMINGHAM METABOLOMICS TRAINING CENTRE

2-4 Nov 2020

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

BIRMINGHAM METABOLOMICS TRAINING CENTRE

5-6 November 2020

Metabolite identification with the Q Exactive and LTQ Orbitrap

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

Overview

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

Topics Covered

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

Course link

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			12-Mar-20		Metabolomics Association of North America Jobs
Research Postdoctoral Scientist	Beaumont Health (Metabolomics Department)	Royal Oak, Michigan, USA	29-Feb-20	Until filled	MetaboNews Jobs
Postdoctoral Research Fellow in Microbial Metabolomics and Natural Products Chemistry	Fundación MEDINA	Granada, Spain	21-Feb-20	Until filled	Fundación MEDINA
Postdoctoral Associate	Yale School of Public Health	New Haven, Connecticut	5-Feb-20	Until filled	Metabolomics Society Job
Senior Bioinformatician	Ann & Robert H Lurie Children's Hospital	Chicago, Illinois, USA	16-Jan-20	Until filled	Ann & Robert H Lurie Children's Hospital
Two Postdoctoral Fellowships	Università Cattolica del Sacro Cuore	Piacenza, Italy	8-Jan-20	Until filled	MetaboNews Jobs
Pos-Doc Fellowship, School of Pharmaceutical Science	University of São Paulo	São Paulo, Brazil	20-Dec-19	Until filled	Metabolomics Society Jobs
Postdoctoral position in Dr. Andres-Lacueva's Group	University of Barcelona	Barcelona, Spain	5-Dec-19	Until filled	Metabolomics Society Jobs

Jobs Wanted

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

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