MetaboNews

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

Metabolomics Society News

Members Corner

Early-Career Members Network (EMN)

EMN Committee Positions

New committee members selected for the 2019-2020 EMN committee will be announced shortly. The EMN would like to thank all of the EMN members who submitted applications for the positions.

EMN Webinars

The EMN hosted the sixth of its series of webinars for 2019. Dr. Gary Siuzdak of the Scripps Research Institute provided an expert perspective titled "Discovering Metabolites that Alter Physiology, an Omics Perspective". Past webinars are available here. Please stay tuned for future EMN webinars.

Metabolites—Open Access Journal

Metabolites (ISSN 2218-1989; Impact Factor: 3.303) is an international, peer-reviewed open access journal of metabolism and metabolomics. It publishes original research articles and review articles in all molecular aspects of metabolism. Our aim is to provide rigorous peer review and enable rapid publication of cutting-edge research to educate and inspire the scientific community worldwide.

Metabolites is indexed by the Science Citation Index Expanded (Web of Science), MEDLINE (PubMed), and other important databases. Manuscripts are peer-reviewed, and a first decision is provided to authors approximately 16.8 days after submission. Acceptance to publication takes approximately 3.5 days (median values for papers published in this journal in the second half of 2018).

The benefits for Metabolomics Society members are as follows:

- **20% discount** on the article processing charge to publish in *Metabolites*
- Discounted publication fees for open access books
- Sciforum.net platform for organizing Metabolomics Society conferences and conference organizing services at preferential rates. Metabolomics Society, as well as each individual member, will be able to use the platform free of charge if self-managed
- The possibility for the society and its members to post job announcements free of charge on the website of *Metabolites*

Associated Special Issue of 2019 Metabolomics Conference in the Hague
More info: https://www.mdpi.com/journal/metabolites/special_issues/Metabolomics2019

10th Anniversary Best Paper Award 2020

Our journal will celebrate its 10th anniversary in 2020. To acknowledge the continued support of our authors, we are pleased to announce the commencement of the Best Paper Awards for research and review articles published from 1 January 2018 to 31 December 2019. Three papers will receive the award, with three papers to be recognized for their quality—the authors of each will receive a certificate, as well as a bonus of 500 CHF and an offer to publish a paper free of charge in *Metabolites*, after the normal peer-review procedure. You can find more details at: http://www.mdpi.com/journal/metabolites/awards/.

Internation Affiliates Corner

Metabolomics South Africa

Visit www.metabolomics-sa.co.za

South African Researchers Introduced to the Field at the National Metabolomics Platform

The 2019 Introductory Metabolomics Workshop was held at the National Metabolomics Platform, based at North-West University's (NWU) Potchefstroom Campus from 5-7 August 2019. This workshop was a collaborative effort between the African Centre for Gene Technologies (ACGT), NWU, and the recently established Metabolomics South Africa (MSA). The workshop provided a capacity building opportunity to help delegates that are in the earlier stages of the research to build a foundation with sound metabolomics techniques and tools.

The workshop was facilitated by a panel of local metabolomics experts from several institutions from all over the country. The facilitators from North-West University were Dr Aurelia Williams, Prof Du Toit Loots, Dr Mari van Reenen, Dr Shayne Mason, Dr Zander Lindeque, Mr Emile Jansen van Rensburg and Ms Zinandre Stander.

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

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info@metabolomicssociety.org
Membership Enquiries
membership@metabolomicssociety.org

The facilitators from the University of Johannesburg included Dr Fidele Tugizimana and Mr Msizi Mhlongo. University of Pretoria was represented by Prof Duncan Cromarty and the University of Cape Town by Dr Zandile Mlamla.

The focus on day one of the workshop was on the different metabolomics workflows, experimental design and the application of metabolomics in different disciplines and industries. On the second day of the workshop the delegates were given an opportunity to participate in real wet lab experiments using NMR and mass spectroscopy. On the final day of the workshop, the focus was mostly on data handling and interpretation. This involved normalization, quality assurance, statistics, metabolite identification, and metabolomics resources.

The participants were from multiple research institutions from all over South Africa. There were participants from the Universities of Pretoria, Johannesburg, the Witwatersrand, Council for Scientific and Industrial Research, North-West University, University of South Africa, Tshwane University of Technology, University of Cape Town, University of Limpopo and the University of KwaZulu-Natal. Below are a few takes offered by the delegates about the workshop:

"The content of the course was well balanced to suite newbies and experienced researchers in metabolomics. It was a great mix of people at different levels of research and different themes which made it rich."

"The course is very insightful to beginners, gives an idea of how to tackle metabolic profiling as well as how to analyse the data. Personally, the course has answered a lot of questions I had, and it inspired me."

"The statistical analysis was extensively covered and will be very useful in considering the best possible statistical tool to use on one's data."

"I enjoyed learning about the different applications of metabolomics and how various types of research questions can be answered through the platform."

"The area of research is still evolving and there is a need to prepare the next generation of researchers for the task ahead to apply it in various fields apart from the human area alone."

"I found the workshop well- structured, comprehensive and rich in content."

The ACGT would also like to wish all the participants of the workshops all the luck with their work and future in metabolomics. Furthermore, the ACGT sends much deserved gratitude to all the members of the organizing committee; Mr Molati Nonyane, Dr Aurelia Williams, Mrs Itseng Malao, Dr John Becker and Dr Fidele Tugizimana for all their efforts in making this event a success.

The ACGT would also like to extend their gratitude to the sponsors of this event: Shimadzu, Microsep, Separations, and the Scientific Group. You are welcome to visit our Facebook page for more visuals from the event.

SpOtlight

METLIN at Half a Million Standards with Experimental ESI-MS/MS Data

Gary Siuzdak
Scripps Center for Metabolomics and Mass Spectrometry

Big Data

Databases are by their nature boring, and METLIN is no different. When originally developed in 2003 METLIN started very modestly with just a few compounds and the acquisition of experimental tandem MS data to facilitate the identification of metabolites. At that time there was simply nothing available that provided this information and we reluctantly undertook the task. METLIN's growth has maintained a relatively steady state in the ensuing 15 years reaching 15,000 molecules with tandem MS data by 2018. However, in 2018 things got a little exciting (by database standards) and METLIN underwent a dramatic expansion. As of August 2019, METLIN has over 500,000 molecular standards with tandem MS data (Figure 1).

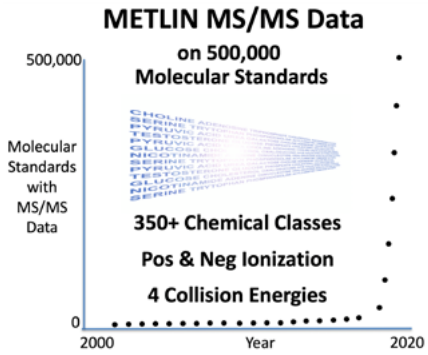

Figure 1. METLIN has gone from thousands of standards with tandem MS data to now over 500,000 standards with tandem MS data since the beginning of 2018.

All the better is that METLIN's data is acquired at four different collisional energies and in both positive and negative ionization modes for each standard. This data now also includes retention time information. When we take into account filtering out low quality data, the total number of individual high-resolution mass data accumulated on the 500,000 standards is 2.4 million tandem mass spectra.

The standards represent 350 different chemical classes including lipids, amino acids, carbohydrates, toxins, small peptides, natural products, drugs, and many other chemical entities. This diversity impacts the identification process in multiple ways. First, the METLIN technology platform is now routinely used for both the identification of known metabolites and other chemical entities. More interesting though, is that it can also be used to identify unknowns specifically through similarity searching.

Similarity Searching

I've always enjoyed the concept of similarity searching, an algorithm originally developed by H. Paul Benton (XCMS2 • Analytical Chemistry 2008). I like it because it is easy to understand and yet can be applied to address one of the most important problems in metabolomics, unknown identification.

The similarity search algorithm was developed to detect structural similarity in unknown metabolites by comparing the unknown's fragment ions (and neutral losses) to tandem MS data contained in METLIN. In its simplest application, fragment similarity searching is performed independent of the precursor mass, relying solely on the fragment ions to identify similar structures within the database (**Figure 2**). Four examples of the identification of previously unknown metabolites were recently demonstrated using METLIN similarity searching, each using more sophisticated techniques (METLIN • Analytical Chemistry 2018). Interestingly, similarity searching for unknown identification was found to be quite valuable when used in conjunction with isotopically labelled compounds.

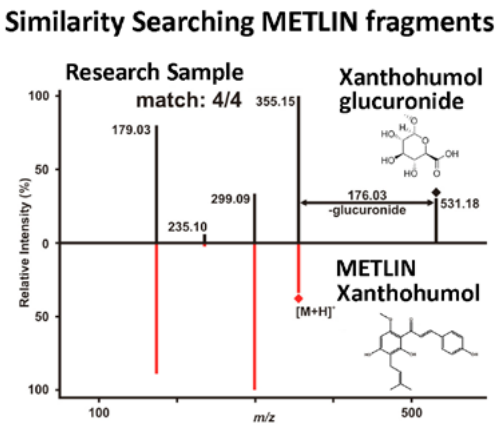

Figure 2. Similarity Searching uses METLIN to help identify unknowns through the similarity of the fragmentation data to the standards tandem MS data. In this case the similarity of xanthohumol data was used to identify its glucuronide conjugate.

Beautiful MISA

Perhaps equal to similarity searching in terms of demonstrating METLIN's utility is MISA or METLIN In-Source fragment Annotation. MISA takes advantage of the surprising abundance of electrospray ionization in-source fragments that occurs and METLIN's low energy collision data. Surprising in that the amount of in-source fragmentation was recently determined to be much more frequent (90%) than anticipated for electrospray ionization (**Annotation • Analytical Chemistry 2018**). METLIN's low energy collision data is key to deciphering the in-source fragmentation providing for identification (**Figure 3**) without using collision-induced dissociation. A clever adaptation of METLIN to turn an annotation problem into an identification advantage by Xavi Domingo et al. (**MISA • Analytical Chemistry 2019**).

Individuals' Contributions to a Greater Whole

This was never solely a Siuzdak thing. I am happy to have started it and shepherded its development. However, the major contributors (all at Scripps) would include Winnie Heim, Aires Aisporna, H. Paul Benton (**Figure 4**), Colin Smith, Theodore Brandon, Emily Chen, Jon Apon, Kevin Cho, Diana Wong, Linh Hoang, Xavi Domingo (METLIN MRM • Nature Methods 2018), and Elizabeth Billings, among others.

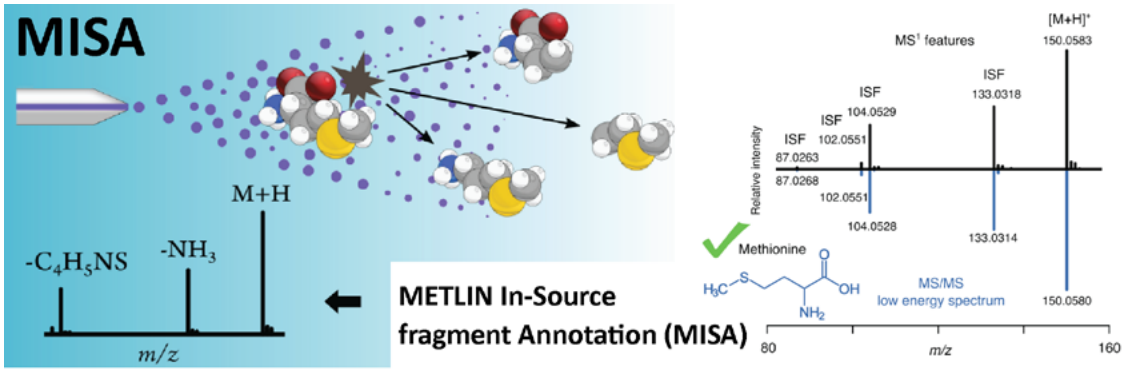

Figure 3. METLIN In-Source fragment Annotation (MISA), an approach that harnesses electrospray ionization in-source fragmentation for rapid molecular identification.

Contributions that included anything from routine data acquisition to intellectual leaps forward in automated data transfer, sample preparation and clever ideas in automated data acquisition and curation (hence the throughput). Curation for example is an integral part of maintaining the quality of METLIN where entries are curated using both automated scripts and manual inspection of the data. Briefly, a script reads the MS files determining charge state and precursor m/z. These are linked with the METLIN entry and a new entry for MS/MS data is initialized in the database. Once this is confirmed the script collects the mass and intensity values for each collision energy (i.e., 0, 10, 20 and 40 V). Finally, the resulting MS/MS data are then subjected to automated and manual (Winnie) inspection before committing it to the database to be viewed on the METLIN site.

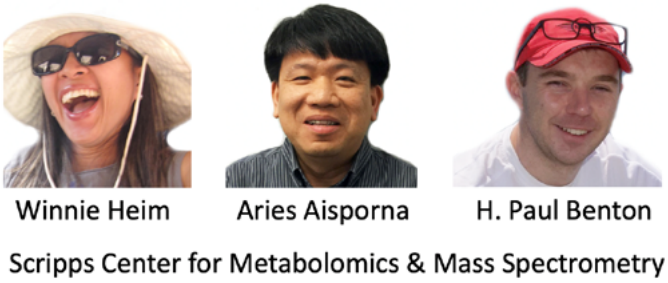

Figure 4. Major METLIN intellectual and data acquisition contributors.

Beyond GC/MS: Broader Implications for Chemical Entity Identification

All details aside, it is worth stepping beyond our metabolomics world for a moment to recognize the broader implications of METLIN. Instead, such an extensive database is a turning point in how we identify molecular entities in general. Instead of relying on GC/MS and its databases that require thermally stable molecules and harsh ionization conditions, rather the METLIN electrospray ionization tandem MS database is the next logical step forward in the evolution of the molecular identification. This is now enabled through the use of standards and the systematic generation of data (pos/neg at four different collision energies), and as we are observing in METLIN's growth, this can be applied to truly large numbers of standards. And perhaps METLIN is much less boring now that the data is here.

Relevant References

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Nature Methods 2018, 15, 681-684.

Recent Publications

Recently published papers in metabolomics

- Use cases, best practice and reporting standards for metabolomics in regulatory toxicology
- Automated Tools for the Analysis of 1D-NMR and 2D-NMR Spectra
- Metformin and Dipeptidase Peptidyl-4 Inhibitor Differentially Modulate the Intestinal Microbiota and Plasma Metabolome of Metabolically Dysfunctional Mice
- Metabolomics for Investigating Physiological and Pathophysiological Processes
- Perspective: Dietaryiomarkers of Intake and Exposure-Exploration with Omics Approaches
- NMR metabolomics: A look ahead
- Beyond the antibodies: serum metabolomic profiling of myasthenia gravis
- MSC-triggered metabolomic alterations in liver-resident immune cells isolated from CCl4-induced mouse ALI model
- New Advances in Amino Acid Profiling in Biological Samples by Capillary Electrophoresis-Mass Spectrometry
- Pre-diagnostic plasma bile acid levels and colon cancer risk: A prospective study

Metabolomics Events

9-13 Sep 2019

5th Metabolomics Sardinian Summer School: "Metabolomics in Cancer Biomarkers and Therapy: Promise and Future"

Venue:
Polaris Technology Park, Pula, Sardinia, Italy

Course Objectives and Targets

Participants will attend theoretical sessions with lectures by experts, and practical sessions to deepen the theoretical and practical knowledge for using the main tools available to better understand the role of metabolism in cancer from a metabolomics point of view. The School is mainly targeted to researchers at an early stage in their career (but not only), from Biological Sciences, Health Sciences and other different background (including Bioinformatics) who are interested in learning about the role of metabolism in cancer by using a metabolomics approach.

Topics Covered

- Analytical approaches in metabolomics: application of MS and NMR
- Metabolite identification
- Data analysis and integration with omics
- Metabolic reprogramming and vulnerability of tumors
- Oncogenes, oncometabolites, and tumor metabolism
- Metabolomics for discovery of new cancer drugs

Applications

The course is funded by the Regional Sardinian government and **registration will be free of charge for all attendees.** Selection will be based on CV and a letter stating the motivations for attending the course and future research plans of candidates. Registration includes course material, lunches and coffee breaks (not accommodation expenses).

Organising Committee

- Atzori Luigi, Università Cagliari, Cagliari , Italy
- Caboni PierLuigi, University of Cagliari, Italy
- Griffin Jules, University of Cambridge, Cambridge, UK
- Pastorelli Roberta, Istituto di Ricerche Farmacologiche Mario Negri, IRCCS, Milano, Italy

Program: http://sites.unica.it/metabolomicaclinica/events/scientific-school-2019/program-2019/

Registration: http://sites.unica.it/metabolomicaclinica/events/scientific-school-2019/

Summer School Contact: latzori@unica.it; metabolomicschool2019@gmail.com

Metabolomics Events

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

24 September 2019

Köln Metabolomics Symposium 2019 - "Red meets green metabolomics"

Venue:
Biozentrum Universität Köln, Köln, Germany

Overview
The first Köln Metabolomics Symposium will be launched under the motto "Red meets green metabolomics", held at the Biozentrum Köln (University of Cologne), Germany on 24 September 2019 from 9.30-18.00 (CET).

This symposium is jointly organized by the University and the University Medical Center of Cologne (CEPLAS, CECAD) and co-organized / supported by BIOCRATES Life Sciences AG, Innsbruck and SCIEX Germany, Darmstadt.

Metabolomics Events

The chairwomen Sabine Metzger and Susanne Brodesser will guide you through two scientific sessions: the "green" session "Plant Metabolomics" will cover various mass spectrometry-based approaches to study plant metabolism. The "red" session "Clinical Metabolomics and Microbiomics" will focus on metabolism and host-microbiome interaction in disease. The recently founded German Society of Metabolomic Research (DGMet) will be introduced as well.

Confirmed Speakers

Susanne Brodesser, Köln • Bijon Chatterji, Innsbruck • Peter Dörmann, Bonn • Fedja Farowski, Köln • Richard Jacoby, Köln • Stephan Krüger, Köln • Daniel Markgraf, Düsseldorf • Sabine Metzger, Köln • Kristina Schlicht, Kiel • Jörg Schlotterbeck, Darmstadt • Martin Späth, Köln • Vivek Venkataramani, Göttingen • Philipp Westhoff, Düsseldorf.

All lectures will be given in English. Please download the detailed programme here. Participation is free of charge, but a pre-registration is recommended (please click the green "Register" button to register).

We are excited to see you in Cologne!

Sabine Metzger, Susanne Brodesser, Petra Blankenstein, Bijon Chatterji
(Organizing committee)

BIRMINGHAM METABOLOMICS TRAINING CENTRE

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

Metabolomics Events

26-27 Sep 2019

6th Munich Metabolomics Symposium: Microbiome Meets Metabolome

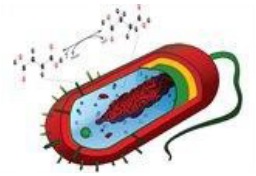
Venue:
Klinikum der LMU München, Munich, Germany

Overview
This scientific symposium seeks to address questions such as:
- How does the microbiome shape host metabolism and contribute to chronic, systemic diseases?
- How to metabolize a microbiome-host to understand and serve as a tool for 'functional microbiome' studies?
- How could 'functional microbiomics' research contribute to the personalized treatment of diseases via nutrition and microbiota directed interventions?

Find the full program of the Symposium here.

Who should attend?
- Researchers with an interest in epidemiology, large cohort studies, and systems biology
- Researchers with an interest in the interplay between microbiota, diseases, treatments, and nutrition
- Researchers with an interest in precision medicine

BIRMINGHAM METABOLOMICS TRAINING CENTRE



9-11 Oct 2019

Introduction to Metabolomics for the Microbiologist

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

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

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

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

Metabolomics Events

21 Oct - 15 Nov 2019

Metabolomics Data Processing and Data Analysis

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

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

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

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

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

25 Oct 2019

Introduction to Metabolomics for the Clinical Scientist

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

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

Metabolomics Events

Topics Covered

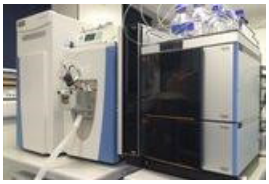
- Introduction to the Phenome Centre Birmingham and the Imperial MRC-NIHR National Phenome Centre showcasing facilities and expertise available.
- Introduction to metabolomics
- Importance of experimental design and sample collection
- Overview of technologies available for data acquisition highlighting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

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

BIRMINGHAM METABOLOMICS TRAINING CENTRE

6-8 Nov 2019

Metabolomics with the Q Exactive



Venue:

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

Overview

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

Topics Covered

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

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

Metabolomics Events

12 Nov 2019

Gunma University Initiative for Advanced Research (GIAR) Exposome Symposium

Venue:
Gunma University, Maebashi, Japan

Overview
This half-day symposium will bring together experts in the exposome field to discuss the latest developments. Talks will focus on the application of high-resolution mass spectrometry in detecting environmental chemicals of concern as well as incorporating exposure data as part of a precision medicine strategy. Registration is free for all attendees.

Confirmed Speakers
Kati Hanhineva, University of Eastern Finland
Douglas Walker, Mount Sinai School of Medicine
Robert Wright, Mount Sinai School of Medicine
Jonathan Martin, Stockholm University
Tracey Woodruff, University of California San Francisco

For registration information and general questions, contact Craig Wheelock
craig.wheelock@metabolomics.se

15-17 Nov 2019

Metabolomics with the Q Exactive

Venue:
Atlanta, Georgia, USA

Overview
Metabolomics researchers from across North America are invited to the first-ever meeting of the Metabolomics Association of North America (MANA) at the Georgia Tech campus in Atlanta, GA, on November 15-17.

The goal of MANA 2019 is to help catalyze more interactions, scientific exchange, and collaboration in the North American metabolomics community. Oral and poster presentation topics will include all sub-disciplines and applications of metabolomics. Additionally, a variety of offerings will focus on trainees and early-career scientists, including lightning talks, social and networking opportunities, and the MANA 2019 Young Investigator Award for excellence in metabolomics work by an early-career scientist.

MANA 2019 will be the premier “big tent“ metabolomics meeting in North America this year, and we look forward to seeing you there! For more information, please visit http://mana2019.org/

Metabolomics Events

BIRMINGHAM METABOLOMICS TRAINING CENTRE

20-21 November 2019

Metabolite identification with the Q Exactive and LTQ Orbitrap

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

Overview

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

Topics Covered

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

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

Metabolomics Jobs & Collaborations

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

Jobs Offered

Job Title	Employer	Location	Posted	Closes	Source
Various Positions			30-Aug-19		Metabolomics Association of North America Jobs
Postdoctoral opportunity, Nutrition and Metabolism/ Biomarkers Group	International Agency for Research on Cancer	Lyon, France	30-Aug-19	30-Sep-19	MetaboNews
Postdoctoral researcher in lipid analytical chemistry	Karolinska Institute	Stockholm, Sweden	29-Aug-19	3-Nov-19	Karolinska Institute
Postdoctoral researcher in metabolomics of respiratory disease	Karolinska Institute	Stockholm, Sweden	29-Aug-19	3-Nov-19	Karolinska Institute
PhD position in plant lipidomics		Bordeaux, France	1-Aug-19	Until Filled	MetaboNews

Jobs Wanted

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

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

- **Seeking New Challenges in Metabolomics**