Metabolomics Society News

Conference Corner

Metabolomics 2019 – The Hague

Thank you for your support for Metabolomics 2019!

We truly thank you for attending the 15th Annual Meeting of the Metabolomics Society at The Hague, the Netherlands.

We reached record-breaking attendance of more than 1000 participants and more than 600 poster and oral presentations. We also can’t thank our sponsors enough for the continuous support in making the Society meeting a great success. We’ll post the photos from the conference on the Society’s website and social media accounts shortly. Please share your fun photos from the conference and tag us.

SAVE THE DATE - Metabolomics 2020

The 16th Annual Conference of the Metabolomics Society will be held in Kerry Hotel Pudong in Shanghai, China, on July 6-10, 2020.

Shanghai is China’s largest industrial and commercial city on China’s east coast and favorite Chinese city for international visitors. The location of Shanghai makes international travel very efficient and convenient for visitors from Europe, North America, and Pacific Ocean countries.

Next year’s Society’s annual conference will put an emphasis on metabolomics (including lipidomics) technology development and the applications in health and disease, medicine (e.g., Chinese traditional medicine), plant science, environment science and other emerging fields.

The meeting will be co-organized with the Chinese Society of Metabolomics (CSM). We will collaborate with international affiliates and industry sponsorships to make available as many travel grants as possible for young scientists. Further details will be released regularly at http://metabolomics2020.org/.

A Call for Abstracts will open in late November/early December. We look forward to seeing you at the inspiring Metabolomics 2020 meeting in Shanghai, China!
Members Corner

Early-Career Members Network (EMN)

EMN Travel Bursary 2019: Winners Announcement!

The Early-career Members Network (EMN) Committee of the Metabolomics Society is pleased to announce the Travel Bursary recipients for 2019.

For the Student Category:

• Maria-Konstantina Ioannidi
  The Institute of Chemical Engineering Sciences, Foundation for Research & Technology – Hellas (FORTH/ICE-HT), Patras, Greece

• Thao V. Nguyen
  The Aquaculture Biotechnology Research Group, Auckland University of Technology (AUT)

For the Postdoctoral Category:

• Oana Zeleznik
  Brigham and Women’s Hospital and Harvard Medical School, Boston, Massachusetts USA

• Caroline Birer
  The University of Pittsburgh, Pennsylvania USA

We thank all applicants with such high-quality applications. Please join us in congratulating the winners who will be awarded $500 to attend conferences in 2019 where they will present their metabolomics-related research.

The EMN Webinar Series 2019

The next EMN webinar series will be held on 17th July 2019 at 14:00 UTC (14:00 GMT, 10:00 EDT, 1:00 AEDT). Dr. Maria Fedorova from Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, University of Leipzig, will present her research expertise on lipidomics and epilipidomics – from analysis to data integration.

She will review current analytical strategies used in contemporary lipidomics and epilipidomics with the focus on optimization of LC-MS/MS based workflows for “discovery” lipidomics including sample preparation, lipid fractionation, separation using different chromatography techniques and high-throughput identification solutions. Available bioinformatics tools for identification of native and modified lipids will be described and compared as well as possible lipidomics data integration strategies.
Dr. Jennifer Kirwan

Head
BIH Metabolomics Platform,
Berlin, Germany

Short Biography

Dr. Kirwan started her career as a clinical veterinarian where she became increasingly interested in how clinical research translated into changes in clinical practice and evidence-based medicine.

After completing her PhD at the University of Liverpool, she moved to the University of Birmingham, UK and from there to the Max Delbrück Center of Molecular Medicine, Germany. She is part of the Berlin Institute of Health (BIH) Initiative to improve translational research and now heads the BIH Metabolomics Platform in Berlin.

This has enabled her to focus on health-related metabolomics and mass spectrometry research and she is particularly interested in the gut-brain-heart health triad.

She is currently involved in several studies which involve long-term sampling and monitoring of individuals and this has led to an interest in appropriate biobanking of samples for metabolomics and lipidomics. She is also a member of the Metabolomics Quality Assurance and Quality Control Consortium (mQACC) and Precision Medicine and Pharmacometabolomics Task Group.
How did you get involved in metabolomics?

I became involved in metabolomics by accident. I was working as a veterinarian at the time, wanted to pursue a PhD and ended up studying a pig disease using metabolomics. I never meant to leave my veterinary roots, but I enjoy what I do and like to think that my work in translational medicine means that I can help many more individuals than I ever could as a practising clinician.

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

We’ve been working hard to improve the automation of the workflow in our lab, and we have just submitted a paper describing software, WiPP, that uses machine learning to improve peak picking for GC-MS.

On the analytical side, we are very interested in the gut microbiome and we have developed a validated quantitative method to measure tryptophan metabolites to help study this. They are involved in so many aspects of health and disease and it’s really exciting to see our hard work in developing and validating this method beginning to yield real results in clinical studies. Both projects were presented at Metabolomics 2019 and we hope will be published later this year.

What is happening in your country in terms of metabolomics?

This is an exciting time to be a Metabolomics Researcher in Germany. We have just founded the German Society for Metabolomics Research, (the Deutsche Gesellschaft für Metabolomforschung, DGMet) (for which I need to acknowledge Jerzy Adamski for all his hard work getting it off the ground). Additionally, the government is currently investing heavily in both translational medicine and mass spectrometry, both of which are areas we are actively working in. The metabolomics and mass spectrometry communities across Germany feel very vibrant at the moment, especially in the field of translational medicine.

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

There is a lot of interest in cardio and vascular health and how it impacts overall health status. We are particularly focused on the gut, heart and brain health axes and how the microbiome interplays with human health. Most of our research is centred on projects relating to these aims and the wider aims of translational medicine.
As you see it, what are metabolomics’ greatest strengths?

Without a doubt, metabolomics greatest asset is its people. It is still a very multidisciplinary subject and seems to attract a diverse crowd of people with a range of skills and backgrounds, who, almost without exception, are highly talented and bring something innovative to the discussion. We work together to solve challenges and to me that's fantastic!

What do you see as the greatest barriers for metabolomics?

I could talk about various technological challenges here, but I think the political barriers also need to be acknowledged. Brexit, trade wars, polarisation of viewpoints; all are pointing towards individual countries becoming less, not more, cooperative. Science works best in a collaborative environment, and if political environments become more hostile to diversity, we will start to lose the benefits that diversity brings. On a positive note, countries that are both well funded and continue to remain open to cooperation and diversity potentially have a lot to gain as they will attract the top scientists to work there.

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

I think metabolomics has really taken off, if the number and scale of requests I am asked to complete are representative. I would like to see us learn from other technological advancements that have gone before us – focus on standardisation, reproducibility and robustness, instrument compatibility and, for the medical field, be realistic about the timescales involved to convert research into practice. Better, quicker and cheaper quantification and identification over a wider range of compounds would be ideal.

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

Currently, funding for metabolomics-based research is good. As metabolomics becomes more mainstream, it will become less likely to attract funding purely for development purposes; instead, it will reflect the overall science funding of the country one resides in. As a community, I think we need to continue to be vocal in the requirement for validation and standardization work so that we know that research is reproducible.

What role can metabolomics standards play?

I see the role of standards as being threefold:

1) **Comparative**: They enable easier comparisons of data from different laboratories and for the reproduction or reuse of data.

2) **Performance quality assurance**: They standardize the expectations of the metabolomics community as to reporting requirements and minimum QA and QC requirements for data to be regarded as valid and robust.

3) **Promoting transparency**: They promote a culture of collaborative and open science by enabling full assessment of methods to be undertaken and the use of data standards that can be easily read and understood by most in the field.

I find it fantastic that we have initiatives such as the Metabolomics Quality Assurance and Control Consortium (mQACC) and the Metabolomics Standards Initiative (MSI) and Core Information for Metabolomics Reporting (CIMR). I hope to see these initiatives converted into a cultural change across the field in both the design of experiments and the reporting culture. As a very basic example, I am still seeing papers being published where metabolomics methods or data processing steps are not being recorded in even a basic manner. This is a significant barrier to someone assessing the results properly or repeating the experiment. As we are often the peer reviewers of such papers, we all have a part of that responsibility in maintaining high-quality reporting as part of maintaining standards in metabolomics.

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

It’s interesting to see the incredible advances made in single cell sequencing in genomics. As the technology advances, I am really excited about the potential of single cell metabolomics to reveal new insight into the development and progression of certain diseases.
Recent Publications

Recently published papers in metabolomics

- A fast, sensitive, single-step colorimetric dipstick assay for quantifying ascorbic acid in urine.

- Herbs and Spices- Biomarkers of Intake Based on Human Intervention Studies - A Systematic Review.

- Protocols for NMR Analysis in Livestock Metabolomics.

- Impact of short-term exposure to fine particulate matter air pollution on urinary metabolome: A randomized, double-blind, crossover trial.

- Metabolomic discrimination of the edible mushrooms Kuehneromyces mutabilis and Hypholoma capnoides (Strophariaceae, Agaricales) by NMR spectroscopy.

- GMSimpute: a generalized two-step Lasso approach to impute missing values in label-free mass spectrum analysis.

- Study on the Potential Biomarkers of Maternal Urine Metabolomics for Fetus with Congenital Heart Diseases Based on Modified Gas Chromatograph-Mass Spectrometer.

- Are we close to defining a metabolomic signature of human obesity? A systematic review of metabolomics studies.

- Deciphering the metabolic perturbation in hepatic alveolar echinococcosis: a 1H NMR-based metabolomics study.

- Towards creating an extended metabolic model (EMM) for E. coli using enzyme promiscuity prediction and metabolomics data.
**Metabolomics Events**

**16-20 September 2019**

The EMBO Practical Course “Metabolomics Bioinformatics in Human Health”

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

**Application Deadline:**
April 15, 2019

**Registration:**

**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
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

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25-27 Sep 2019

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

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

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

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

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

9-13 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
**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](https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/introduction-metabolomics-microbiologist.aspx)
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 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

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

25 Oct 2019

Introduction to Metabolomics for the Clinical Scientist

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

Overview
This one-day course in partnership with the Phenome Centre Birmingham provides clinicians with an overview of the metabolomics pipeline highlighting the benefits of this technique to the medical field and an introduction to the Phenome Centre Birmingham and the MRC-NIHR National Phenome Centre.

The course provides a suitable introduction to metabolomics prior to taking additional training courses at either the Birmingham Metabolomics Training Centre or the Imperial International Phenome Training Centre.
Metabolomics Events

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

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

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**6-8 Nov 2019**

**Metabolomics with the Q Exactive**

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

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

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

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

20-21 November 2019

Metabolite identification with the Q Exactive and LTQ Orbitrap

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

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

Topics Covered
• Importance of mass spectral interpretation
• Types of data which can be collected on the QE and LTQ-Orbitrap (m/z, retention time, MS/MS, 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](https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/metabolite-identification.aspx)
### Jobs Offered

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<td>Montreal, Quebec, Canada</td>
<td>11-Jun-19</td>
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<td>Tier 2 CIHR Canada Research Chair (CRC) in Clinical Omics and Diagnostics</td>
<td>Technion – Israel Institute of Technology</td>
<td>Haifa, Israel</td>
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<td>PhD and postdoctoral fellow positions in Metabolomics and Lipidomics</td>
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<td>Grand Rapids, Michigan, USA</td>
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<td>Postdoctoral position in mass spectrometry</td>
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<td>3-Jun-19</td>
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<td>Icahn School of Medicine at Mount Sinai</td>
<td>New York, New York, USA</td>
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<td>3-Apr-19</td>
<td>Until filled</td>
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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 (metabolomics.innovation@gmail.com). Upon review, a limited number of job submissions will be selected for publication in the Jobs Wanted section.

- There are currently no listings