Metabolomics Society News

Conference Corner

Call for Expressions of Interest (EOI) to host the 2021 Metabolomics Conference in Americas

The Metabolomics Society is calling for interested members in the Americas to express their interest in hosting the 2021 annual Metabolomics Society meeting. Please send notice of your interest using this form by 30 January 2019.

You should name individuals who will be key to forming a Local Organizing Committee (LOC) and outline the scientific plan for the conference. The LOC will report to the Metabolomics Society and assist A-S-K staff to select a suitable venue and organize the conference. The tasks of the LOC are to ensure national and regional support for the conference, to assist the Society in administrative planning and, most importantly, to chair and organize the scientific management of the conference, including forming an International Organizing Committee that is responsible for scientific aspects of the meeting.

Please complete the application form outlining your ideas to maximize the scientific quality and outreach of the conference. For further enquiries, please contact the Society via A-S-K Associates (metabolomics@askusa.com).

Following receipt of the EOIs, the Metabolomics Society Conference Committee will determine which groups are asked to submit full proposals. Templates for full proposals will be sent in February 2019 and will be due in May 2019.

Metabolomics 2019 – The Hague

Planning for the 15th Annual Conference of the Metabolomics Society is underway; look for registration to open in December! Call for Workshops is currently open, the deadline has been extended to January 7, 2019. Find the form online: http://www.metabolomics2019.org/
Members Corner

Early-Career Members Network (EMN)

EMN Webinar Series:

The EMN is planning to establish a series of online webinars from 2019 onwards. Please stay tuned for our upcoming webinars. You can access the recorded videos of the past webinars on the Metabolomics Society website.

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EMN Bursary Program:

Follow the EMN on facebook (https://www.facebook.com/EMN.MetabolomicsSociety/) for the upcoming call 2019 and apply for our travel grant to expand YOUR horizon!

Please feel free to contact us via info.emn@metabolomicssociety.org if you have any suggestions on our activities or additional ideas that the EMN could organize.
Réseau Français de Métabolomique et Fluxomique (RFMF)

The RFMF board, the RFMF junior and the local committees are happy to announce the organization of the 12th Scientific Conference of RFMF taking place in Clermont-Ferrand from May 21st to May 23rd 2019. A satellite event will take place May 20th 2019 and will be dedicated to workshops and round tables. This 12th edition will again be the opportunity to stimulate exchanges within the French-speaking community by offering 4 plenary talks by internationally speakers, oral presentations, 180 seconds flash presentations, thematic and poster sessions.

International renowned speaker venue is already confirmed

- Coral Barbas (University of San Pablo Madrid)
- Pieter Dorrestein (University of California)
- Claudio Luchinat (University of Florence)
- Konstantinos A. Aliferis (University of Athens)

RFMF will promote methodological and technological developments for metabolomics, fluxomics, lipidomics and volatilomics with new:

- Analytical developments
- Data pre- and post-processing
- Statistics and data integration

Both English and French will be spoken during the conference.

Main thematic research areas covered during the 12th RFMF conference will be applications of metabolomics and fluxomics in the areas of:

- Nutrition
- Environment
- Pharmacology/toxicology
- Plants
- Health
- Food product quality
- Biotechnologies

There will be the opportunity for RFMF to award several prizes during the conference proceedings: PhD award 2019, poster prizes and best flash presentation.

We hope that the conference will continue to provide a friendly atmosphere for networking within the French-speaking Community.
MetaboAnalyst provides a user-friendly, web-based analytical pipeline for high-throughput metabolomics studies. MetaboAnalyst specifically aims to offer a variety of commonly used procedures for metabolomic data processing, normalization, multivariate statistical analysis, and data annotation. The current implementation focuses on exploratory statistical analysis, functional interpretation, and advanced statistics for translational metabolomics studies.

MetaboAnalyst 4.0 now contains a total of 12 modules organized into four general categories:

- **Exploratory statistical analysis**: general statistics, biomarker analysis, two-factor/time-series analysis, and power analysis
- **Functional enrichment analysis**: metabolite set enrichment analysis, metabolic pathway analysis, and pathway activity prediction from MS peaks (mummichog)
- **Data integration and systems biology**: biomarker meta-analysis, joint-pathway analysis, and network explorer
- **Data processing and utility functions**: compound ID conversion, batch effect correction, lipidomics, and links to several spectra analysis tools

It accepts a variety of metabolomics data types, as well as a list of genes or KEGG orthologs (KOs) to support integrative analysis with transcriptomics or metagenomics respectively.

**Data Formats:**
MetaboAnalyst supports diverse data formats from metabolomic studies including compound concentrations, NMR/MS spectral bins, NMR/MS peak intensity table, NMR/MS peak lists, and LC/GC-MS spectra. For more details about the various formats, visit the [Data Formats](#) page.

**Data Processing:**
Depending on the type of the uploaded data, different data processing options are available (see [details](#)). This is followed by data normalization steps including normalization by constant sum, normalization by a reference sample/feature, sample specific normalization, auto/Pareto/range scaling, etc.
Statistical Analysis:
A wide array of commonly used statistical and machine learning methods are available:
- Univariate: fold change analysis, t-tests, volcano plot, and one-way ANOVA, and correlation analysis
- Multivariate: principal component analysis (PCA), partial least squares-discriminant analysis (PLS-DA) and orthogonal partial least squares-discriminant analysis (Orthogonal PLS-DA)
- High-dimensional feature selection: significance analysis of microarrays (and metabolites) (SAM) and empirical Bayesian analysis of microarrays (and metabolites) (EBAM)
- Clustering: dendrogram, heatmap, K-means, and self-organizing map (SOM)
- Supervised classification: random forests and support vector machine (SVM)

Functional Enrichment Analysis:
The service performs metabolite set enrichment analysis (MSEA) for human and mammalian species. It can accept a list of compound names, a list of compound names with concentrations, or a concentration table. The analysis is based on several libraries containing ~6300 groups of biologically meaningful metabolite sets collected primarily from human studies.

Metabolic Pathway Analysis:
The service currently supports pathway analysis (including pathway enrichment analysis and pathway topology analysis) and visualization for 21 model organisms, including human, mouse, rat, cow, chicken, zebrafish, Arabidopsis thaliana, rice, Drosophila melanogaster, malaria, budding yeast, E. coli, etc., with a total of 1600 pathways.

Time Series and Two-Factor Data Analysis:
The service currently supports clustering and visualization (including interactive 3D PCA visualization and two-way heatmaps with hierarchical clustering), two-way ANOVA for univariate two-factor analysis, multivariate empirical Bayes time-series analysis (MEBA) for detecting distinctive temporal profiles across different experimental conditions, and ANOVA-simultaneous component analysis (ASCA) for identification of major patterns associated with each experimental factor (and their interactions).

Biomarker Analysis:
The service provides receiver operating characteristic (ROC) curve-based approach for evaluating the performance of potential biomarkers. It offers classical univariate ROC analysis and more modern multivariate ROC curve analysis based on PLS-DA, SVM, or Random Forests. In addition, users can manually pick biomarkers or set up hold-out samples for flexible evaluation and validation.

To Try MetaboAnalyst
Click Here

Useful Links:
- FAQs
- Tutorials
- Troubleshooting
**Sample Size and Power Analysis:**
Users can upload a dataset either from a pilot study or from a similar study to compute the minimum number of samples required to detect the effect within a certain degree of confidence and to estimate the power of the current study design.

**Joint Pathway Analysis:**
The service allows users to simultaneously analyze genes and metabolites of interest within the context of metabolic pathways. Only data from human, mouse, and rat are supported currently.

**MS Peaks to Pathway Activities:**
Users can upload LC-MS peaks to perform metabolic pathway enrichment analysis and visual exploration based on the well-established **mummichog** algorithm. It currently supports 21 organisms including human, mouse, zebrafish, C. elegans, and other species.

**Network Explorer:**
Users can upload one or two lists of metabolites, genes, or KEGG orthologs (i.e., generated from metagenomics), and then visually explore these molecules of interest within the context of biological networks such as KEGG global metabolic network and several networks created based on known associations between genes, metabolites, and diseases.

**Biomarker Meta-Analysis:**
Users can upload several metabolomics data sets obtained under comparable conditions to identify robust biomarkers across multiple studies. It currently supports meta-analysis approaches based on p-value combination, vote counts, and direct merging. The results can be explored in interactive Venn diagram.

**Image Generation:**
Important images can be re-produced in high resolution in various format such as Portable Network Graphics (.png), Tagged Image File Format (.tiff), PostScript (.ps), etc., for publication purposes.

**Report Generation:**
Upon completion, a comprehensive PDF report will be generated documenting each step performed along with corresponding tabular and graphical results. The processed data and images are also available for download.

**Referencing MetaboAnalyst:**


Recent Publications

Recently published papers in metabolomics

- A Simple and convenient synthesis of unlabeled and 13C-Labeled 3-(3-Hydroxyphenyl)-3-hydroxypropionic acid and its quantification in human urine samples.

- A sensitive, high-throughput LC-MS/MS method for measuring catecholamines in low volume serum.

- A review on human fecal metabolomics: Methods, applications and the human fecal metabolome database.

- Vegetable signatures derived from human urinary metabolomic data in controlled feeding studies.

- Headspace gas monitoring of gut microbiota using targeted and globally optimized targeted secondary electrospray ionization mass spectrometry.

- Lipidomic response to coffee consumption.

- Effects of gut bacteria depletion and high-Na+ and low-K+ intake on circulating levels of biogenic amines.

- Changes in the serum metabolite profile correlate with decreased brain gray matter volume in moderate-to-heavy drinking young adults.

- Plasma metabolite profiles in healthy women differ after intervention with supplemental folic acid v. folate-rich foods.

- Urinary metabolomics reveals novel interactions between metal exposure and amino acid metabolic stress during pregnancy.
**16-18 Jan 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

30 Jan-1 Feb 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
3-8 Feb 2019

Understanding Human Diseases Through Metabolomics: Interactions Among the Genome, Proteome, Gut Microbiome and Nutrition (Gordon Conference Series on Metabolomics and Human Health)

Venue:
Four Points Sheraton / Holiday Inn Express
1050 Schooner Drive
Ventura, CA, USA

Application Information

Applications for this meeting must be submitted by January 6, 2019. Please apply early, as some meetings become oversubscribed (full) before this deadline. If the meeting is oversubscribed, it will be stated here. Note: Applications for oversubscribed meetings will only be considered by the conference chair if more seats become available due to cancellations.

Conference Description

Metabolomics is the comprehensive study of the metabolome, the repertoire of biochemicals present in cells, tissues, and body fluids. The study of metabolism at the global or “-omics” level is a rapidly growing field that has the potential to have a profound impact upon medical practice. At the center of metabolomics, is the concept that a person’s metabolic state provides a close representation of that individual’s overall health status. This metabolic state reflects what has been encoded by the genome, and modified by diet, environmental factors, the gut microbiome among other influences. The metabolic profile provides a quantifiable readout of biochemical state from normal physiology to diverse pathophysilogies in a manner that is often not obvious from gene expression analyses. In this Gordon Conference series, we highlight state of the art metabolomics technologies and their applications to the study of human health and disease.

We will cover most recent developments in the field covering applications of metabolomics for deeper understanding of disease mechanisms, disease heterogeneity and disease progression; variation in treatment outcomes and enablement of precision medicine approaches; connections between metabolome, proteome and genome and atlases being created; effects of exposome, diet and gut microbiome on human metabolome and health. We will highlight large consortia initiatives which enable epidemiology and clinical studies, functional genomics, nutrigenomics, pharmaceutical applications including toxicology studies, systems pharmacology, environmental exposures effects on health (exposome) and beyond. We invite established as well as early career members to attend this meeting from academia industry and regulatory agencies.

For further information, please visit:
Metabolomics Events

25 Feb to 1 Mar 2019

Hands-on NMR Spectroscopy for Metabolic Profiling

Venue:
Imperial College London, Exhibition Road, 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, NMR spectrometer set up for global profiling, 2-dimensional NMR experiments and spectral data analysis.

Earlybird: £1750
Standard: £1950
Registration: Register using this link

For further information and registration details, please visit http://www.imperial.ac.uk/imperial-international-phenome-training-centre/courses/hands-on-nmr-spectroscopy-for-metabolic-profiling/

28 Feb-1 Mar 2019

Introduction to Metabolomics for the Environmental Scientist

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

Overview
This two-day NERC-funded Advanced Training Short Course provides environmental scientists with an overview of the metabolomics pipeline. The course is intended for environmental scientist with little or no previous experience of metabolomics and who are interested to discover how this relatively new and powerful approach could be integrated into their research. Experts working in the NERC Metabolomics facility NBAF-B will teach the course.

Topics Covered
• Introduction to environmental metabolomics with case studies
• Experimental design and quality control
• Sample collection and preparation
• Overview of analytical laboratory techniques (mass spectrometry and NMR spectroscopy)
• Short practical demonstrations and a tour of the metabolomics facilities
• Overview of data processing and statistics for metabolomics
• Introduction to metabolite identification
• Q&A session with an opportunity for course leads to provide advice on your own metabolomics studies

Course Link
https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/introduction-metabolomics-environmental.aspx
Introduction to Metabolomics for the Clinical Scientist

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

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

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

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

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

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

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

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

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

For further information, please visit http://www.cpsa-metabolomics.com/2019/index.shtml.
Overview
Structure determination of molecules contained within unresolved complex mixtures represents an unsolved question that continues to challenge physical and analytical chemistry. Most naturally occurring systems can be characterised as complex mixtures. These can be broadly divided according to the molecular sizes of their constituents, into mixtures of small or large molecules. The focus of this Faraday Discussion will be on the former, while the latter such as biomacromolecules, industrial polymers, or solid matrices are outside of its scope as such. Nevertheless, the processes that are used in analysing the data originating from these studies may be of interest.

Examples of small molecule mixtures include:
- Environmental matrices such as soil, dissolved organic matter, organic molecules contained in atmospheric aerosol particles, or crude oil
- Biofluids
- Man-made mixtures of small molecules such as food, beverages or plant extracts

These systems are generally classed as “complex mixtures” or “unresolved complex mixtures (UCM)”, emphasising our current inability to separate their individual components.

The techniques best positioned to tackle such mixtures experimentally include mass spectrometry, chromatography, NMR spectroscopy, or new alternative techniques, including combinations of the above methods. For the most part, people who work on the analysis of complex mixtures are driving the progress in exploiting new methodologies and their creative combinations.

For further information and registration details, please visit http://www.rsc.org/events/detail/29574/challenges-in-analysis-of-complex-natural-mixtures-faraday-discussion
### Jobs Offered

<table>
<thead>
<tr>
<th>Job Title</th>
<th>Employer</th>
<th>Location</th>
<th>Posted</th>
<th>Closes</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>PhD in Metabolomics (BBSRC iCASE with Unilever)</td>
<td>University of Birmingham</td>
<td>Birmingham, United Kingdom</td>
<td>30-Nov-18</td>
<td>6-Jan-19</td>
<td>FindAPhD</td>
</tr>
<tr>
<td>Various Positions</td>
<td></td>
<td></td>
<td>6-Dec-18</td>
<td></td>
<td>Metabolomics Association of North America</td>
</tr>
<tr>
<td>Postdoctoral Fellow in Metabolomics and Exposomics</td>
<td>Icahn School of Medicine at Mount Sinai</td>
<td>New York, USA</td>
<td>21-Sep-18</td>
<td>Until filled</td>
<td>Metabolomics Society Jobs</td>
</tr>
<tr>
<td>Postdoctoral Fellow</td>
<td>National Institutes of Health</td>
<td>Bethesda, Maryland, USA</td>
<td>9-Nov-18</td>
<td>Until filled</td>
<td>Metabolomics Society Jobs</td>
</tr>
<tr>
<td>Postdoctoral researcher in Metabolomics, Synthetic Biology and Metabolic Engineering</td>
<td>University of Luxembourg</td>
<td>Belvaux, Luxembourg</td>
<td>29-Oct-18</td>
<td>31-Dec-18 or until filled</td>
<td>University of Luxembourg</td>
</tr>
<tr>
<td>Assistant Professor in Chemistry</td>
<td>University of Nebraska-Lincoln</td>
<td>Lincoln, Nebraska, USA</td>
<td>10-Oct-18</td>
<td>Until filled</td>
<td>Metabolomics Society Jobs</td>
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</table>

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