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Metabolomics Society News

Members Corner

Board of Director Election

Thank you for your participation in the Board of Director Election in August! We are pleased to announce the results of the election and welcome some new faces to the Board:

Re-elected for another two-year term: Jules Griffin, Krista Zanetti, Nichole Reisdorph, Oliver Jones, Christophe Junot, Justin van der Hooft, and Craig Wheelock.

Newly joining the Board for a two-year term: Caroline Johnson, Jessica Lasky-Su, Dan Raftery, and Ralf Weber. We also welcome Isabel Orf to the Board as the Chair of the EMN for the next year.

Early-Career Members Network (EMN)

New EMN Committee Announcement

The EMN Committee is pleased to announce its eight new members: Corey Giles (Australia), Elena Legrand (USA), Fatema Bhinderwala (USA), Julia Maria Malinowska (UK), Jun Zhou (USA), Katharina Herzog (Sweden), Natasa Giallourou (UK), and Patrick Trainor (USA). Congratulations!

They will join four committee members who will continue their term for a second year: Christina Jones (USA), Dara Daygon (Australia), Isabel Orf (UK), and Umaporn Uawisetwathana (Thailand). Krista Zanetti will continue her role as the EMN Advisor; Charmion Cruickshank-Quinn will join her in an advisory role as Past Chair. We also greatly thank outgoing committee members who did very great jobs last year: Ricardo Heredia (UK) and Zhanlong Mei (Denmark). We are looking forward to working with all the new committee members to continue developing our activities through webinar series, conference workshops, and new outreach activities for early-career members.

EMN Bursary Program

To view the conference reports from two of the winners of the travel grants, visit: <https://drive.google.com/open?id=1fTu3YT2z5f2cwYOeuJjh6luFZ0KyHV4n>

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

Metabolomics News

Mexico City Prospective Study

Between 1998 and 2004, CTSU (Clinical Trial Service Unit), in collaboration with the Mexican Ministry of Health, established a study in Mexico City, in which over 150,000 middle-aged adults (including 100,000 women and 50,000 men) provided information about their lifestyle and disease history, had physical measurements recorded (including weight, waist and hip circumference, blood pressure) and had a blood sample taken.

All participants are now being tracked for mortality through linkage to Mexican national mortality databases; by January 2016, about 20,000 were confirmed to have died. By relating participants' characteristics at recruitment to death over the following decades, this study is now investigating the main environmental and biological causes of premature death in Mexico.

A resurvey of 10,000 surviving participants (2015 - 2018) captured how lifestyles, physical and biological measurements and treatments for disease (e.g. diabetes) have changed over time. The resurvey also allowed us to better assess the relevance to premature death of characteristics that can vary over time (such as adiposity, diabetes, blood pressure, smoking and alcohol consumption). It also included various 'enhancements' (such as bioimpedance, lung function and the collection of a urine sample).

The Mexico City Prospective Study offers an opportunity to study within a single large cohort the social, lifestyle, physical, metabolic and genetic causes of disease in a Latin-American population.

The study is being done in collaboration with the National Autonomous University of Mexico in Mexico City and has received funding from the Mexican Ministry of Health (Secretaria de Salud), the Mexican National Council of Science and Technology (Consejo Nacional de Ciencia y Tecnología), the British Heart Foundation, the UK Medical Research Council, and the UK Wellcome Trust (grant number 058299/Z/99).

Nightingale Health will perform metabolic profiling of the Mexico City Prospective Study cohort by analysing the biomarker profiles of blood samples from the 150,000 study participants.

Biomarker profiling technology measures metabolic biomarkers that recent studies have found to be predictive of future risk for heart disease, type 2 diabetes and many other common chronic diseases. Until recently, technological constraints and prohibitive costs have prevented the analysis of comprehensive biomarker data from large-scale population collections. The new technology makes this viable by measuring over 220 metabolic biomarkers from a single blood sample. Nightingale will perform the assays within 12 months allowing researchers to start investigating the novel dataset promptly.

Biomarker profiling will allow us to better understand how lifestyle, environment and genetics combine to cause diseases such as cardiovascular disease in a population with high levels of obesity and diabetes.

Source: <https://www.ctsu.ox.ac.uk/research/prospective-blood-based-study-of-150-000-individuals-in-mexico>



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

General Enquiries

info@metabolomicsociety.org

Membership Enquiries

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PhenoMeNal: An Online Portal for Metabolomics

August 30 Hinxton – An international collaboration between EMBL's European Bioinformatics Institute (EMBL-EBI) and 13 other partners has made large-scale metabolomics analyses easier with the launch of [PhenoMeNal](#).

This online portal allows researchers and clinicians to analyse large metabolomics datasets. For example, researchers can search for patterns in a patient's data, and use the findings to improve the detection of disease and to help optimise treatment. This project has received funding from the European Union's Horizon 2020 research and innovation programme.

Source: <https://www.ebi.ac.uk/about/news/press-releases/PhenoMeNal-metabolomics>

SpOtlight

Structure Elucidation of Unknown Metabolites by Combined NMR and MS/MS Prediction

Rene M. Boiteau¹, David W. Hoyt¹, Carrie D. Nicora¹, Hannah A. Kinmonth-Schultz², Joy K. Ward² and Kerem Bingol¹

¹Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington, USA

²Department of Ecology and Evolutionary Biology, University of Kansas, Lawrence, Kansas, USA

Identification of unknown metabolites is the central bottleneck of untargeted metabolomics research. Traditionally, identification of unknown metabolites has been performed by extensive isolation of the molecule from extracts in sufficient amount for detailed analysis by MS, NMR, X-ray, circular dichroism and other analytical techniques. While this approach has been proven useful, complete fractionation is time-consuming. Moreover, low yield of purification may not allow downstream structure elucidation process for low-abundance metabolites. Alternatively, structure elucidation can be performed in the mixture environment, such as in crude extracts or partially fractionated samples.

There are three main approaches proposed for unknown identification in mixtures; the first approach uses only mass spectrometry techniques. This approach compares experimental fragmentation spectra of an unknown metabolite with the predicted fragmentation of all possible candidate isomeric structures to find the best match. The second strategy, on the other hand, only relies on NMR, where the experimental chemical shifts of unknown metabolites are sequentially assigned and deconvoluted by multidimensional NMR. These assignments are further verified through comparison against their quantum NMR chemical shift predictions.

While these MS- and NMR-based approaches greatly facilitate the structural characterization, they have limited power, since they rely only on a single technique. Recently, several hybrid MS/NMR metabolite identification strategies have been proposed.

One of our latest hybrid NMR/MS techniques, ISEL NMR/MS2 (Integrated Structure ELucidation by NMR/MS2) is a novel approach that combines *in silico* MS/MS and NMR predictions into a single analysis platform to improve accuracy of automated unknown metabolite identification. In this approach, the unknown metabolites are first identified by determining their chemical formula from high resolution LC-MS1 spectrum. Next, all feasible candidate structures consistent with the chemical formula are generated by using a structure generator. MS/MS and NMR spectra of each candidate structures are predicted and compared with the experimental MS/MS and NMR spectra of the same sample, and finally ranked according to the level of agreement to determine the best matching candidate.

Metabolite	Formula	Size ^a	MS/MS rank ^b	NMR rank ^c	NMR rank ^d
Phenylalanine	C ₉ H ₁₁ NO ₂	1881	1	2	2
Valine	C ₅ H ₁₁ NO ₂	453	6	1	1
Nicotinate	C ₆ H ₅ NO ₂	100	7	1	1
Pantothenate	C ₉ H ₁₇ NO ₅	563	8	4	16
Glutamine	C ₅ H ₁₀ N ₂ O ₃	283	10	1	1
Methionine	C ₅ H ₁₁ NO ₂ S	212	13	1	1
Isoleucine	C ₆ H ₁₃ NO ₂	962	22	1	1
Proline	C ₅ H ₉ NO ₂	528	26	2	2
Thymidine	C ₁₀ H ₁₄ N ₂ O ₅	948	40	2	2
Leucine	C ₆ H ₁₃ NO ₂	962	148	1	3

Table 1. MS/MS and NMR results for ten commonly known metabolites.

^a Number of structures for a given molecular formula (obtained with ChemSpider); ^b rank-ordered agreement between experimental and predicted MS2 of a given metabolite (obtained with MetFrag); ^c rank-ordered agreement between predicted and experimental chemical shifts of a given metabolite when the metabolite was the only unknown in the NMR spectrum; ^d rank-ordered agreement between predicted and experimental chemical shifts of a given metabolite when the metabolite was one of the ten unknowns in the NMR spectrum.

We first compared the performances of MS/MS and NMR predictions on a mixture of ten commonly known metabolites (Table 1). Based on these comparisons, NMR predictions turned out to be a more effective filter than MS/MS predictions. However, MS/MS predictions provided an orthogonal method that allowed to distinguish between molecules that yield similar NMR chemical shifts. Thus, combining NMR and MS/MS predictions further improved the accuracy of metabolite identification.

As a real-world example, we applied the ISEL NMR/MS2 approach on identification of an uncatalogued secondary metabolite in *Arabidopsis thaliana* extract, which allowed successful identification of glucoraphanin, a type of glucosinolate in *Arabidopsis* (Figure 1).

In the glucoraphanin example in Figure 1, that considered one unknown metabolite at a time, the NMR spectrum was paired with a single LC-MS feature by an offline LC fractionation procedure. However, it is also common in metabolomics to analyze complex mixtures consisting of multiple metabolites within unfractionated samples. In these cases, multiple LC-MS features and multiple deconvoluted NMR spectra are generated, without knowing which pairs correspond to the same metabolite. This increases the challenge of high-throughput metabolite identification in mixtures.

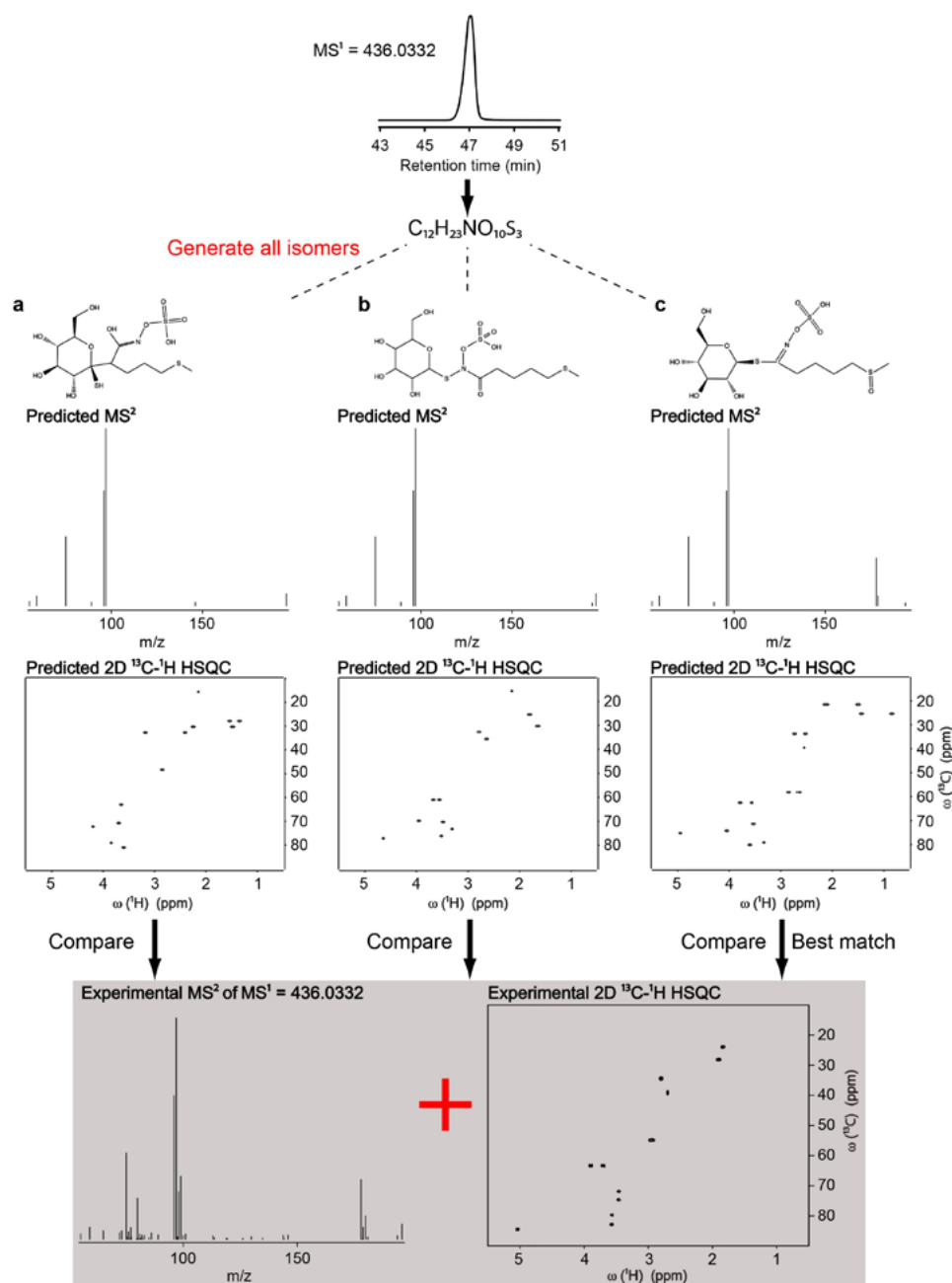


Figure 1. Illustration of the workflow of the ISEL NMR/MS² approach on identification of glucoraphanin in *Arabidopsis* extract. Chemical formula of the unknown metabolite was first determined from high resolution LC-MS¹ spectrum. Next, all feasible candidate structures consisted with the chemical formula were generated. MS/MS and NMR spectra of each candidate structures were predicted and compared with the experimental MS/MS and NMR spectra of the same sample, and ranked according to the level of agreement to determine the best matching candidate.

In cohort studies MS and NMR features can be paired by statistical correlation. Unfortunately, for the analysis of a single sample, statistical correlation is not an option. In this case, the ISEL NMR/MS2 approach can still be applied. When multiple unknowns are present, the workflow is modified to consider all pairwise combinations; NMR predictions are generated for all structural isomers of each LC-MS feature (chemical formula), and they are all compared to every deconvoluted experimental NMR spectra of the mixture.

Proof-of-principle was demonstrated on the ten-compound mixture. In 8 out of 10 cases, the rank orders of metabolite identifications did not increase from being the only metabolite in the NMR spectrum to being one of the ten metabolites in the mixture (Table 1). Overall, these results showed that the ISEL NMR/MS2 approach is promising for the identification of real unknowns in mixtures.

Literature reference

Boiteau, RM.; Hoyt, DW.; Nicora, CD.; Kinmonth-Schultz, HA.; Ward, JK.; Bingol, K. "Structure Elucidation of Unknown Metabolites in Metabolomics by Combined NMR and MS/MS Prediction" *Metabolites* **2018**, 8, 8.

<http://www.mdpi.com/2218-1989/8/1/8>

Acknowledgement

This work was performed at Environmental Molecular Sciences Laboratory, a national scientific user facility sponsored by DOE's Office of Biological and Environmental Research and located at Pacific Northwest National Laboratory (PNNL). PNNL is operated by Battelle for the DOE under Contract DE-AC05-76RL01830.

The banner features the ChenomX logo on the left, which consists of a dark green circle with a yellow dot above the word "CHENOMX" in white. To the right of the logo, the text "NMR ANALYSIS YOU CAN TRUST" is displayed in white. Below the logo, the website "www.chenomx.com" is shown in white text on a yellow rectangular background. The background of the banner is a blurred image of laboratory glassware, including vials and a beaker. In the bottom right corner, there is a screenshot of the ChenomX software interface, showing a chemical structure of Aspartic acid and its corresponding NMR spectrum with peaks labeled.

Recent Publications

Recent Publications

Recently published papers in metabolomics

- [Metabolic profiling of human plasma reveals the activation of 5-lipoxygenase in the acute attack of gouty arthritis.](#)
- [Integrated Pharmacodynamic Analysis Identifies Two Metabolic Adaption Pathways to Metformin in Breast Cancer.](#)
- [Nutrition and prevention of cognitive impairment.](#)
- [Proteomics, metabolomics and metagenomics for type 2 diabetes and its complications.](#)
- [Metabolomics in the Clinic: A Review of the Shared and Unique Features of Untargeted Metabolomics for Clinical Research and Clinical Testing.](#)
- [Plasma lipid profiling of tissue-specific insulin resistance in human obesity.](#)
- [Biomarkers of dementia in obstructive sleep apnea.](#)
- [Mechanism of YLTZ on glycolipid metabolism based on UPLC/TOF/MS metabolomics.](#)
- [Untargeted metabolomics: an overview of its usefulness and future potential in prenatal diagnosis.](#)
- [Byproduct Generated During the Elaboration Process of Isotonic Beverage as a Natural Source of Bioactive Compounds.](#)

Metabolomics Events



11-13 Nov 2018

Lipidomics Forum

Venue:

Dortmund, Germany

The fourth Lipidomics Forum is being hosted between the 11th and 13th of November 2018 at ISAS in Dortmund, which is a joint effort with the Research Center Borstel. This symposium is an annual series of conferences on lipid biology and lipidomics to provide a platform for international acknowledged scientists, students, and young researchers to interact.

Specifically, we will encourage students to participate by poster presentations and short talks allowing them to receive advice from experts in the field. Therefore, this symposium series will not only cover current research highlights but also offer tutorials on selected methodical topics. We are convinced to have created a stimulating and scientifically attractive fourth edition of the Lipidomics Forum especially for you.

For this year, the German society for mass spectrometry ([DGMS](#)) offers travel grants for Ph.D. students (200€ within North Rhine-Westphalia, otherwise 250€), at most three grants per work group.

For further information and registrations details, please visit:

<https://lipidomics-forum.isas.de/index.php>



Metabolomics Events



15-30 Nov 2018

The 3rd International Electronic Conference on Metabolomics

Venue:
Online

The 3rd International Electronic Conference on Metabolomics will be held online (<https://sciforum.net/conference/iecm-3>) from **15–30 November 2018**, enabling you to present your latest research to the scientific community and to have the opportunity to participate in fruitful exchanges of information with academic and industrial groups from all over the world. It is absolutely **FREE of charge** to participate as an author or a visitor; all you need to do is register on the home page. After the conference, the authors are also welcome to submit an extended version of the proceeding papers to the [Special Issue](#) of Journal *Metabolites* with a **20% discount** off the Article Processing Charge.

Main Topics

- Advanced Metabolomics and Data Analysis Approaches
- Identification of Unknowns
- Precision Nutrition and Food Specific Profiles
- Microbiota and Metabolomics
- Pathway Mapping and Fluxomics

Key Dates

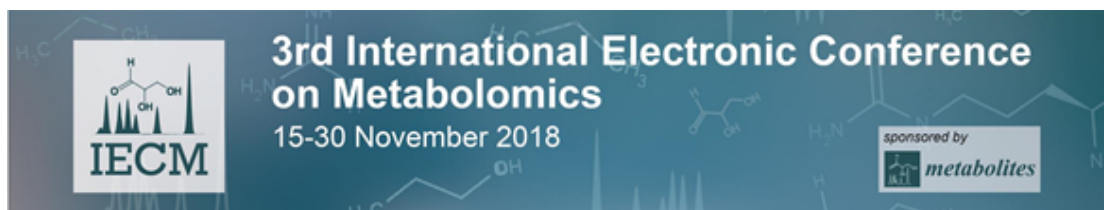
25 September, 2018 Deadline for Abstracts

This year, as a sponsor, *Metabolites* would like to award the best presentation as selected by an evaluation committee. The winner will be offered publication of the extended full manuscript free of charge in the Special Issue of *Metabolites* together with a Certificate.

We look forward to receiving your contributions.

For more information and to register, please visit:

<https://sciforum.net/conference/iecm-3> and follow us on Twitter [@MetabolitesMDPI](#).



Metabolomics Events



19-21 Nov 2018

Metabolomics with the Q Exactive

Venue:

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

This 3-day course will introduce you to using the Q Exactive mass spectrometer in your metabolomics investigations. The course is aimed at students and researchers with minimal previous experience of applying LC-MS in metabolomics. The course will be led by experts in the field and include lectures, laboratory sessions and computer workshops to provide:

- An introduction to metabolomics and using the Q Exactive mass spectrometer in your studies
- Polar and non-polar sample preparation for profiling and targeted studies
- Data acquisition for profiling and targeted studies
- Data processing and data analysis
- Introduction to metabolite identification

The course will finish with a question and answer session with a panel of experts.

For further information and registrations details, please visit <http://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/introduction-metabolomics.aspx> or contact bmtc@contacts.bham.ac.uk



22-23 Nov 2018

Metabolite identification with the Q Exactive and LTQ Orbitrap

Venue:

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

Limited bursaries are now available for PhD students funded by NERC, which make the registration for this course **FREE** to these students.

This 2-day course will provide a hands-on approach to teach the latest techniques and tools available to perform metabolite identification. We will apply these tools on the Q Exactive and LTQ Orbitrap mass spectrometry family. The course is targeted towards students and researchers who are actively applying metabolomics.

The course will be led by experts in the field and include significant hands-on experience using both the Q Exactive and LTQ Orbitrap instruments to perform:

- Data dependent acquisition
- Data independent acquisition
- MS/MS and MSⁿ data acquisition

The course will finish with a session on the tips and tricks from the experts and an opportunity to ask questions.

For further information and registration details, please visit <http://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/metabolite-identification.aspx> or contact bmtc@contacts.bham.ac.uk

Metabolomics Events

Imperial College
London

27-30 Nov 2018

Hands-on Data Analysis for Metabolic Profiling

Venue:

Imperial College London, Exhibition Road, 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.

Earlybird: £900 (valid until 15 October 2018)

Standard: £1100

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-data-analysis-for-metabolic-profiling/>

Imperial College
London

3-7 Dec 2018

Hands-on LC-MS 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, the use of mass spectrometry for global profiling and targeted methodologies and data analysis.

Earlybird: £1750 (valid until 22 October 2018)

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-lc-ms-for-metabolic-profiling/>



Metabolomics Events

Imperial College
London

3-7 Dec 2018

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/>

MetaboMeeting
2018 17-19 December
University of Nottingham, UK

17-19 Dec 2018

Metabomeeting 2018

Venue:

University of Nottingham, United Kingdom

Welcome to MetaboMeeting 2018. The Metabolic Profiling Forum is delighted to announce the 11th Metabomeeting which is to be held at the University of Nottingham in the UK on the 17th-19th December 2018.

The meeting will bring together research scientists and practitioners from all areas of application and development of metabolic profiling, covering a wide range of experience from early career scientists to experts from throughout the international metabolomics field.

MetaboMeeting 2018 continues to highlight the work of its attendees through both oral platform presentation and poster sessions.

Oral presentation and poster abstract submission 30 September 2018

For further information and registration details, please visit:

http://thempf.org/mpf_cms3/index.php

Metabolomics Events



31 Jan - 30 June 2019

Research Hotel Application

Venue:

The Metabolomics Innovation Centre. Edmonton, Canada

Application deadline is Sept. 30 2018

The Metabolomics Innovation Centre (TMIC) at the University of Alberta, in Edmonton, Alberta, Canada offers hands-on training opportunities in metabolomics and bioinformatics to qualified scientists. To apply, [please complete the application here](#).

For more information, contact dchamot@ualberta.ca.



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 pathophysiologies 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:

<https://www.grc.org/metabolomics-and-human-health-conference/2019/>

Metabolomics Events

Imperial College
London

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/>

UF Clinical and Translational
Science Institute
UNIVERSITY of FLORIDA

11-13 March 2019

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>.

Metabolomics Events



13-15 May 2019

Challenges in Analysis of Complex Natural Mixtures Faraday Discussion

Venue:

John McIntyre Conference Centre, University of Edinburgh, 18 Holyrood Park Road, Edinburgh, EH16 5AY, United Kingdom

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>

Metabolomics Jobs & Collaborations

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

Jobs Offered

Job Title	Employer	Location	Posted	Closes	Source
Postdoctoral Researcher Position	UCSF	San Francisco, USA	01-Mar-18	Until filled	Metabolomics Society Jobs
Senior Scientific Officer (Lipidomics/ Metabolomics)	Nanyang Technological University	Singapore	12-Feb-18	Until filled	Metabolomics Society Jobs
Postdoc Position in Cheminformatics and Computational Metabolomics	Friedrich-Schiller-University	Jena, Germany	09-Feb-18		Friedrich-Schiller-University
Ph.D. Position on Mass Spectrometry-Based Analysis of Metabolites	University of Basel	Basel, Switzerland	31-Jan-18	Until filled	Metabolomics Society Jobs
Various Positions			25-Sep-18		Metabolomics Association of North America
Postdoctoral Fellow in Metabolomics and Exposomics	Icahn School of Medicine at Mount Sinai	New York, USA	21-Sep-18	Until filled	Metabolomics Society Jobs
Research Scientist, Chemistry	Driscoll's	Watsonville, California, USA	26-Sep-18	30-Nov-18	Metabolomics Society Jobs
Postdoctoral Fellow in Metabolomics and Exposomics	Icahn School of Medicine at Mount Sinai	New York, NY, USA	21-Sep-18	Until filled	Metabolomics Society Jobs
Multiple bioinformatics positions	Emory University	Atlanta, GA, USA	17-Sep-18	Until filled	Metabolomics Society Jobs
PhD in Clinical Metabolomics, Metabolomics Unit, Faculty of Biology and Medicine	University of Lausanne, Switzerland	Lausanne, Switzerland	30-Aug-18	Until filled	Metabolomics Society Jobs
Senior Research Assistant in Metabolomics	Icahn School of Medicine at Mount Sinai	New York, USA	24-Jan-18	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.
