MetaboNews

JANUARY 2019
Vol 9 Issue 1

In This Issue

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

Metabolomics Society News

Conference Corner

Registration for Metabolomics 2019 is open!

The 15th Annual Conference of the Metabolomics Society will be in The Hague, The Netherlands from June 23-27, 2019, in the World Forum conference centre in The Hague. This jubilee edition is expected to draw a record number of participants, making it the largest Society meeting to date. On June 23-24, 2019, we will see a new high of 18 pre-conference workshops, offering an ideal learning opportunity for early-career scientists.
New elements to the programme are an additional six Introduction to the Field sessions where leading PIs give an overview of their field in small-scale interactive sessions and Career Night on Sunday June 23. At Career Night, employers from academia and industry are posting their job openings, giving the opportunity to early-career and more experienced researchers looking for a next step in their career to meet in person in an informal setting. Several career-related workshops will be taking place during this time.

The conference itself will focus on the applications of metabolomics in academia and industry. The plenary keynote lectures will be given by researchers, not necessarily performing metabolomics analyses themselves, but rather they use and integrate metabolomics in their lines of research. We especially encourage early-career researchers to participate in Metabolomics 2019, and therefore we expect a record number of travel grants will be available, as well as a conference mobile app.

The call for abstracts for posters and oral presentations will open shortly, please keep an eye on the website of the conference http://www.metabolomics2019.org/. The website will be continuously updated, with the latest confirmed speakers and workshops. We would like to welcome you all to The Hague in June 2019. And last but not least: the complimentary conference dinner will be at a Beach Club!

Jules Griffin
Metabolomics Society President

Board of Directors

Words From the President

Firstly, I would like to wish everyone a Happy New Year and hope to see many of you at the World Forum in the Hague, the Netherlands for this year's International Meeting of the Metabolomics Society (June 23-27, 2019). Preparations are well under way and if you want to find out more please take a look at: http://metabolomics2019.org/. The local organising committee led by Merlijn van Rijswijk, Robert Hall, and Thomas Hankemeier have put in a huge amount of groundwork and we should be shortly announcing our Plenary and Keynote speakers. However, the majority of speaking slots are available through the abstract submission process, and this year there are more slots than in any other previous meetings so I encourage you to start thinking about what you would like to present. There will also be poster sessions.

I would also like to reiterate a warning that seems to also come around this time of the year. We are currently plagued by several rogue conferences, also claiming to be International conferences involving metabolomics, often with the words systems biology or omics in their title. These conferences try to entice registrations by offering 'keynote speaking slots' or the request to organise a session to what they claim is an international meeting but is often just a hotel meeting room. There is one story I was told recently where a presenter was asked to chair his own session which just consisted of fellow speakers, including chairing his own Q&A session, which is not the experience anyone wants when you have spent time and money attending a meeting. If you are in any doubt about the veracity of a meeting please contact the Board of the Society who would only be too happy to confirm whether a conference is genuine or not. Alternatively, you can check whether the conference is listed in MetaboNews or on the Society's website as we vet all of these meetings.

Meanwhile, I'm going to get back to my data processing – hopefully there's an abstract in there!

Jules Griffin

Members Corner

Early-Career Members Network (EMN)

EMN Webinar Series:

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

EMN Bursary Program 2019: Application Announcement!

EMN bursary program provides support to early-career scientists (including graduate students and post-docs) to attend national and international events related to the metabolomics field. Early-career scientists will be able to apply for a bursary ($500) towards the cost of travel and conference/event fees.

METABOLOMICS SOCIETY

METABOLOMICS SOCIETY
EARLY-CAREER MEMBERS NETWORK

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

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

Save the date for your application:

- January 31st – applications open
- February 28th - deadline of application
- April – notification of winners

New to metabolomics or stuck with a problem? We recommend Metabolomics wiki and Metabolomics Forum. Follow us on Twitter (@MetabolomicsSoc) and Facebook (EMN.metabolomicssociety) to stay up-to-date on all news and upcoming events.

Task Groups Corner

Industry Engagement Task Group

We are looking for individuals to become part of and to help re-invigorate the INDUSTRY TASK GROUP. Individuals from industry, academia, government, or any other interested person is welcome to join! Our first meeting will be scheduled for February 2019 and we will be meeting approximately monthly thereafter.

We are hoping to have a standing committee of 6-12 individuals plus at least one representative from interested companies who is willing to attend at least two meetings per year. Our first job as a committee will be to determine a set of broad goals and specific tasks to accomplish in 2019. We will also be coming up with two, three, and five-year plans. As a member of this group, you can expect to commit anywhere from 2-5 hours per month. We will also plan a face-to-face meeting at the annual meeting and will invite you to attend a VIP event at the annual meeting. Please check your email for more information, including a list of tentative goals. Please email Nichole at Nichole.Reisdorph@UCDenver.edu for more information or to join.

International Affiliates Corner

Australian & New Zealand Metabolomics Network (ANZMN). (Visit http://www.anzmn.org)

The ANZMN would like to wish all our members and their families a very happy New Year. We hope 2019 is a good one for you all!

SpOtlight

The MxP® Quant 500 Kit

A Quantitative, Broad-Coverage Metabolomics Kit Targeting Host-Microbiota Interactions

Barbara Wolf, Svenja Heischmann, Stephen Dearth, and Therese Koal

BIOCRATES Life Sciences AG, Innsbruck, Austria

Metabolomics links Microbiome to Systemic Diseases and Therapy Response

Research findings on the symbiotic relationship of microbiota and host have dramatically reshaped our understanding of human physiology and the impact of microbes on pathophysiological processes[1]. In particular, the gut microbiota plays an immense role in the host's physiology including energy homeostasis, synthesis of essential vitamins (B and K), stimulation as well as regulation of the immune system, defense against pathogens, removal of toxins, digestion including fermentation of dietary fibers into short-chain fatty acids (SCFA, e.g., acetic and butyric acid), and metabolization of small molecules (e.g., bile acids, sterols, and xenobiotics). Mediated by microbiota-derived metabolites, communication channels such as the gut-liver axis (via e.g., branched chain amino acids and bile acids), gut-brain axis (e.g., serotonin, gamma-amino butyric acid), and gut-immune axis (e.g., indoles, taurine) regulate interactions between the gut and the respective organ.

Knowledge about functional microbiome-host interactions, including its homeostatic balance, has led to new insights into the pathogenesis of chronic systemic diseases such as diabetes, non-alcoholic fatty liver disease, and cancer (Figure 1).

In addition, responses to therapies, for instance chemotherapy, may be dependent on the microbiome[2].

While gene sequencing provides information on microbial diversity in the gut, metabolomics is the analytical technique of choice to assess microbial functions which shape the metabolic phenotype. At least 10% of endogenous metabolites found in blood are derived directly from the gut microbiota[3]. Many of these metabolites produced by gut bacteria are derived from dietary components (e.g., SCFA, indoles, polyamines) or biochemical modifications of endogenous metabolites (e.g., secondary bile acids, taurine)[4].

To investigate host-microbiota crosstalk, we have recently introduced the MxP® Quant 500 kit. This standardized assay provides the most comprehensive analytical coverage of metabolites and lipids in kit format. It enables targeted metabolomics analysis delivering reproducible, quality-controlled quantitative data of up to 630 metabolites and lipids. Thereof, numerous provide insight into the connection of the gut microbiota and nutrition to the host, offering a holistic picture of an individual's phenotype.

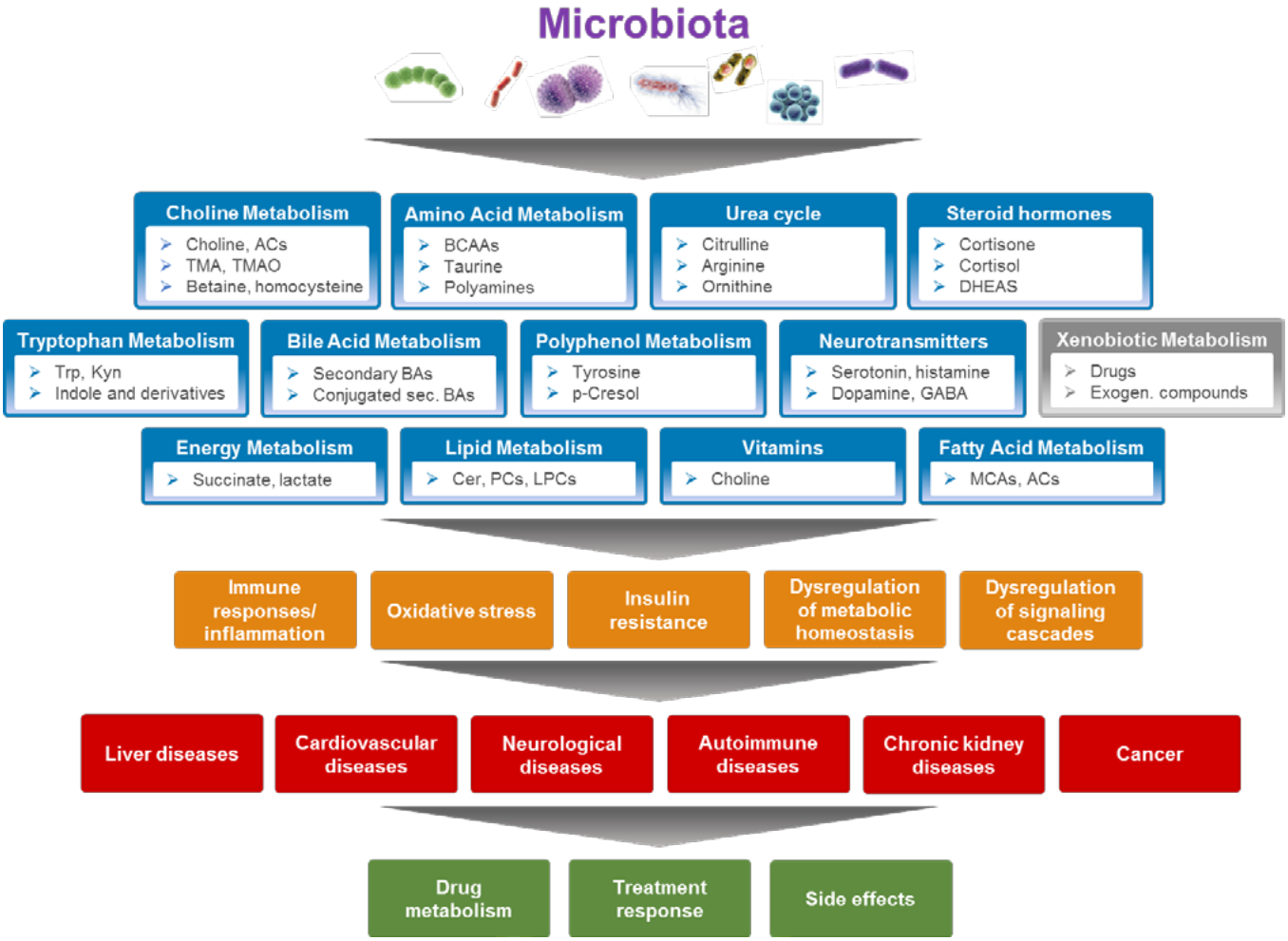


Figure 1: Schematic representation of influences of the microbiota on metabolism, health status, and therapy. The MxP® Quant 500 kit captures 630 metabolites and lipids (exemplary analytes are represented in blue boxes) connecting the microbiome to metabolic conditions (exemplary events in orange boxes), resulting pathophysiology (red boxes), and treatment of diseases (green boxes). Abbreviations: ACs, acylcarnitines; BAs, bile acids; BCAAs, branched-chain amino acids; Cer, ceramides; DHEAS, dehydroepiandrosterone; GABA, gamma-aminobutyric acid; Kyn, kynurenine; LPCs, lysophosphatidylcholines; MCAs, medium chain fatty acids; PCs, phosphatidylcholines; Trp, tryptophan.

The MxP® Quant 500 Kit

The MxP® Quant 500 kit, the latest addition to Biocrates' kit portfolio, is a targeted metabolomics assay that enables multiplexed analysis of up to 630 metabolites and lipids from 14 small molecule and 12 lipid classes using a sample volume of only 10uL. The standardized format of the assay ensures the generation of quantitative, quality-controlled results, which are especially important when conducting longitudinal or inter-laboratory studies. Sums and ratios can easily be calculated from the quantitative data for biological data interpretation.

The MxP® Quant 500 kit was developed specifically for use with ultra-high-performance liquid chromatography/triple quadrupole mass spectrometry (UHPLC-MS/MS). The kit is currently available for SCIEX triple quadrupole MS/MS instruments; support for additional manufacturers' (U)HPLC platforms will be available soon. The 96-well plate format allows for the analysis of up to 80 samples per kit besides calibration standards and quality control samples. The ready-to-use kit includes reagents, a filter plate with pre-loaded internal standards, our proprietary workflow manager software Met*IDQ*™, and a detailed user manual.

Key features of the Met*IDQ*™ software:

- Guided workflow: sample registration, plate layout and instrument sample worklists generation, and data validation
- Assisted system suitability test
- Ready-to-use instrument-specific data acquisition methods
- Automated metabolite and lipid identification and quantification
- Tools for data normalization across plates and batches

The MxP® Quant 500 kit has been specifically designed and validated for use with human plasma. It has also been successfully applied to the analysis of other matrices such as human feces and rat plasma (for more information, please refer to the product page).

The numbers of detected metabolites and lipids in each sample are mainly dependent on the biological matrix: in-house we were able to detect ~455 metabolites in human plasma, ~440 in the standard material NIST 1950 (human plasma), ~415 in rat plasma, and ~120 in human feces (Table 1). Optimization of the sample preparation protocol for human feces prior to using the kit may yield higher numbers of detected metabolites and lipid as sample preparation conditions affect recovery of fecal metabolites and lipids.

The MxP® Quant 500 Kit in Microbiome Research:

The MxP® Quant 500 kit is the first metabolomics kit developed for research on host-microbiome interactions covering both host- and microbiota-derived metabolites. Metabolites of all central pathways are captured by the kit (Figure 2). In the following, three selected metabolic pathways are described in more detail.

Many metabolites of **choline and betaine metabolism** are supplied by food and can be metabolized by gut bacteria[5]. Betaine (trimethylglycine, TMG) primarily results from the oxidation of dietary choline in mitochondria, mainly in liver and kidneys. Betaine may contribute to a reduction of toxic homocysteine levels in blood, thereby reducing the risk for atherosclerosis, depression, cognitive decline, and liver damage. Choline, carnitine, and betaine can be metabolized by gut bacteria to trimethylamine (TMA), which can be converted to trimethylamine N-oxide (TMAO) by liver enzymes. High circulating levels of TMAO are associated with insulin resistance and cardiovascular disease. A shift in choline metabolism towards high betaine levels with concomitant reduction of TMAO may be beneficial for systemic metabolic health. Therefore, supplementation with associated compounds, such as betaine, may be used therapeutically to prevent chronic diseases.

Analyte Class	Total	Human Plasma	Rat Plasma	Human Feces	NIST 1950
Alkaloids	1	0	1	1	1
Amine Oxides	1	1	1	0	1
Amino Acids	20	20	20	18	20
Amino Acid Related	30	19	22	14	20
Bile Acids	14	13	13	13	13
Biogenic Amines	9	3	7	7	3
Carbohydrates and Related	1	1	1	0	1
Carboxylic Acids	7	3	4	1	2
Cresols	1	1	1	1	1
Fatty Acids	12	5	5	8	5
Hormones and Related	4	2	0	0	2
Indoles and Derivatives	4	3	3	2	3
Nucleobases and Related	2	1	0	2	1
Vitamins and Cofactors	1	1	1	1	1
Acylcarnitines	40	17	15	2	14
Glycerophospholipids (Lysophosphatidylcholines and Phosphatidylcholines)	90	76	76	9	76
Sphingomyelins	15	14	14	1	15
Cholesteryl Esters	22	18	17	4	16
Ceramides	28	15	9	12	16
Dihydroceramides	8	1	0	1	1
Glycosylceramides (Mono-, Di-, and Trihexosylceramides)	34	19	9	6	13
Diglycerides	44	8	5	7	6
Triglycerides	242	214	189	7	211
Total	**630**	**455**	**413**	**117**	**442**

Table 1: Typical numbers of metabolites and lipids detected with the MxP® Quant 500 kit according to the tested biological matrices.

**Use of different homogenization protocols prior to using the kit may yield higher numbers of detected metabolites and lipids. Applied homogenization protocol (ethanol phosphate buffer-based) was optimized for small molecule analysis.*

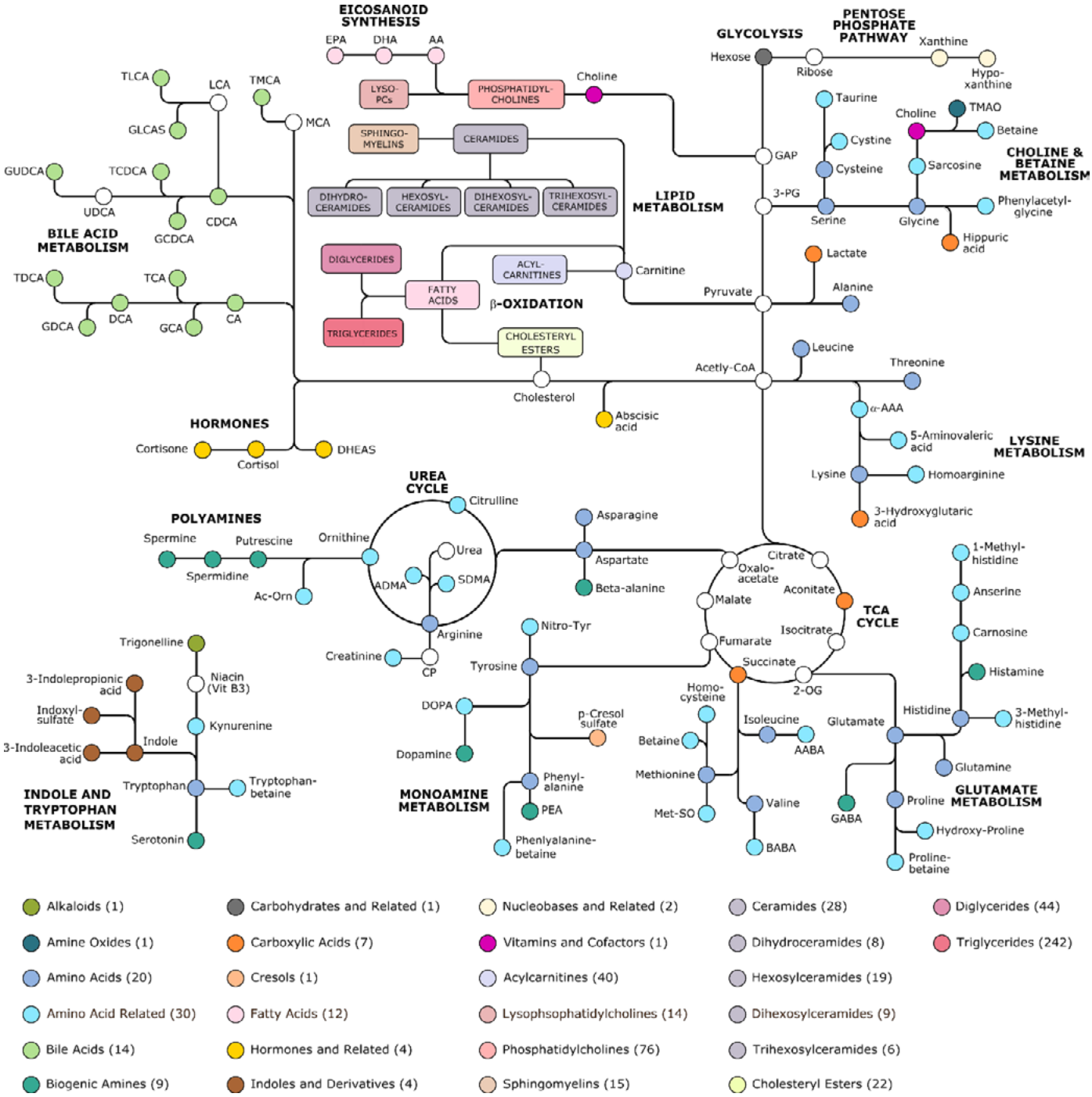


Figure 2: Overview of the metabolic pathways covered by the MxP® Quant 500 kit. The numbers in parentheses represent the numbers of metabolites or lipids assessible within the respective analyte classes.

The gut microbiota regulates three major pathways of tryptophan metabolism: indole, kynurenine, and serotonin pathways[6]. Dietary tryptophan can be converted by the gut microbiota into indoles and aryl-hydrocarbon receptor (AhR) ligands that regulate local and distant functions in host metabolism, including immune homeostasis and gut barrier integrity. The gut microbiota also influences the kynurenine-generating enzyme indoleamine 2,3-dioxygenase (IDO). This enzyme plays a critical role in inflammation, immune responses, and in the central nervous system. In addition, gut-produced serotonin has many local and distant effects, such as on gut motility and central serotonergic pathways.

Bile acid metabolism plays an important role in host physiology besides the digestion of dietary fats[7]. Bile acids are end products of cholesterol metabolism. Originally produced in the liver, stored as bile in the gall bladder, and shed to the small intestine, bile acids undergo enterohepatic recirculation several times per day. Gut bacteria convert primary to secondary bile acids, which may exert cytotoxic effects. In recent years, the role of bile acids as important signaling molecules (e.g., via the farnesoid X receptor, FXR) has been elucidated to regulate processes such as glucose metabolism, innate immunity, as well as cell growth and differentiation.

Consider the MxP® Quant 500 kit if you are interested in:

- Targeting the worldwide broadest metabolite and lipid coverage
- A standardized, ready-to-use kit format ensuring outstanding analytical robustness as well as longitudinal and inter-laboratory comparability
- Exploring host-microbiome interactions

For more information on the **MxP® Quant 500 kit**, please visit the product page.

To access the Biocrates literature database, please register here.

References

1. Gentile CL, Weir TL. The gut microbiota at the intersection of diet and human health. Science 2018;362:776–80.

2. Zitvogel L, Ma Y, Raoult D, Kroemer G, Gajewski TF. The microbiome in cancer immunotherapy: Diagnostic tools and therapeutic strategies. Science 2018;359:1366–70.

3. Wikoff WR, Anfora AT, Liu J, et al. Metabolomics analysis reveals large effects of gut microflora on mammalian blood metabolites. Proc Natl Acad Sci U S A 2009;106:3698–703.

4. Postler TS, Ghosh S. Understanding the Holobiont: How Microbial Metabolites Affect Human Health and Shape the Immune System. Cell Metab. 2017;26:110–30.

5. Griffin JL, Wang X, Stanley E. Does our gut microbiome predict cardiovascular risk? A review of the evidence from metabolomics. Circ Cardiovasc Genet 2015;8:187–91.

6. Agus A, Planchais J, Sokol H. Gut Microbiota Regulation of Tryptophan Metabolism in Health and Disease. Cell Host Microbe 2018;23:716–24.

7. Long SL, Gahan, Cormac G M, Joyce SA. Interactions between gut bacteria and bile in health and disease. Mol Aspects Med 2017;56:54–65.

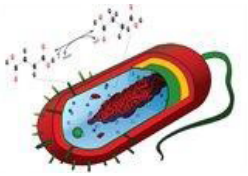
Recent Publications

Recently published papers in metabolomics

- BioTransformer: a comprehensive computational tool for small molecule metabolism prediction and metabolite identification
- CEU Mass Mediator 3.0: a metabolite annotation tool
- PAIRUP-MS: Pathway analysis and imputation to relate unknowns in profiles from mass spectrometry-based metabolite data
- Integrative analysis of blood metabolomics and PET brain neuroimaging data for Parkinson's disease
- Identification of Unknown Metabolomics Mixture Compounds by Combining NMR, MS, and Cheminformatics
- Metabolomics discloses potential biomarkers to predict the acute HVPG response to propranolol in patients with cirrhosis
- Investigation of the relationships between knee osteoarthritis and obesity via untargeted metabolomics analysis
- Recent advances and perspectives of metabolomics-based investigations in Parkinson's disease
- Association between serum haptoglobin and carotid arterial functions: usefulness of a targeted metabolomics approach
- Alteration of Metabolic Pathways in Osteoarthritis

Metabolomics Events

BIRMINGHAM METABOLOMICS TRAINING CENTRE



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

Metabolomics Events

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

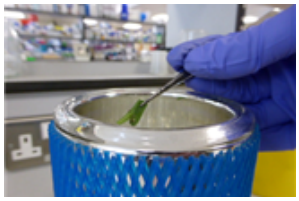
Venue:
Imperial College London, Exhibition Road, London, United Kingdom

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/

BIRMINGHAM METABOLOMICS TRAINING CENTRE



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

Metabolomics Events

11 Mar 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.

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

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

1-3 April 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

4-5 April 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.

Metabolomics Events

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

ROYAL SOCIETY OF CHEMISTRY

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

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

Metabolomics Events

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

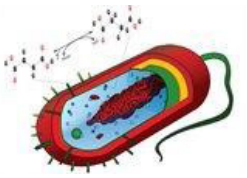
Overview
This three-day course provides a theoretical overview and hands-on training to apply multiple sample preparation and UPLC-MS methods to characterise the metabolomes of complex biological samples using the mass spectrometer (Xevo QToF G2-XS - a maximum of 4 people working on the instrument in 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

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.

Metabolomics Events

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

BIRMINGHAM METABOLOMICS TRAINING CENTRE

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.

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

Metabolomics Events

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 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			16-Jan-19		Metabolomics Association of North America
Postdoctoral position in metabolomics as applied to the studies of traumatic brain injury	Örebro University	Örebro, Sweden	15-Jan-19	10-Feb-19	Örebro University
Analytic-Specialist in Cell Culture Research (M/F)	Roche	Penzberg, Bavaria, Germany	9-Jan-19	Until filled	Metabolomics Society
Ph.D. Position on Mass Spectrometry-Based Analysis of Drug Metabolites	University of Basel	Basel, Switzerland	26-Dec-18	Until filled	Metabolomics Society
Tier 2 Canada Research Chair in Biomedical Metabolomics	Queen's University	Kingston, Ontario, Canada	20-Dec-18	Until filled	Metabolomics Society
Postdoctoral Fellow in Epigenetics and Cellular Metabolism	Van Andel Research Institute	Grand Rapids, MI USA	11-Dec-18	Until filled	Van Andel Research Institute
Postdoctoral Fellow	National Institutes of Health	Bethesda, Maryland, USA	9-Nov-18	Until filled	Metabolomics Society Jobs
Postdoctoral Fellow in Mass Spectrometry and Exposomics	Icahn School of Medicine at Mount Sinai	New York City, NY USA	31-Jan-2019	Spring 2019	Metabolomics Association of North America
Associate Researcher Position in Mass Spectrometry and Exposomics	Icahn School of Medicine at Mount Sinai	New York City, NY USA	31-Jan-2019	Spring 2019	Metabolomics Association of North America

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.