Workshop Details

WORKSHOP SCHEDULE

SUNDAY, JUNE 25			
Workshops at University of Queensland St. Lucia			
	Sir James Foots Building 47A - 341	**Sir James Foots Building 47A - 241**	**Hawken Building Room 50-T203**
13:00 - 15:00	**Workshop 1:** MetaboTools: Analysis of metabolomic data in the context of the metabolic model	**Workshop 2:** ANZMET Round Table + Peer Sessions	**Workshop 3:** EMN Workshop - Experimental Design in Metabolomics
15:00 - 15:30	**Break**		
15:30 - 17:30	**Workshop 1 Continued:** MetaboTools: Analysis of metabolomic data in the context of the metabolic model	**Workshop 4:** Network medicine approaches for the analysis of metabolomics data	**Workshop 5:** EMN Workshop - MS Metabolomics Data Processing

MONDAY, JUNE 26			
Workshops at BCEC			
	M1	**M2**	**M3**	**M4**
8:00 - 19:00	**Registration is Open**			
8:45 - 10:15	**Workshop 6:** Hybrid Ion Mobility MS	**Workshop 7:** Role of Metabolomics for Health & Diet Research	**Workshop 8:** Data Sharing, Standardisation and Workflow for reproducible analysis in Metabolomics	**Workshop 9:** EMN Workshop - Statistical Considerations and Pathway Analysis Strategies
10:15 - 10:30				
10:30 - 12:00	**Workshop 10:** Advances in High Throughput Targeted Metabolomics Analysis	**Workshop 11:** EMN Workshop - Career Development	**Workshop 12:** Metabolite Identification Annotation	**Workshop 13:** Clinical Biomarker Detection

Metabolomics 2017 will begin Monday afternoon, following Workshops.
See Conference Agenda for the complete schedule.

There is not a registration desk at University of Queensland on Sunday.
Pick-up your registration materials on Monday morning at the BCEC.

How to get to the Sunday Workshops – June 25

Workshops on Sunday afternoon will take place at the University of Queensland (UQ) in St Lucia. Most workshop meeting rooms are located in the Sir James Foots building (building 47A), however the (2) EMN workshops are located in the Hawken Building, Room 50-T203 (Raybould Lecture Theatre).

Public transport options to UQ include:

- Bus 66 from Cultural Centre Busway Station (BCEC), South Bank Busway Station (South Bank Area), or King George Square Station (City Centre); traveling to UQ Lakes Station.

    o About 15 mins travel time from Cultural Centre, runs every 15 mins.

    o Last bus to catch to be on time for the workshops: 12:09pm King George Sq., 12:13pm Cultural Centre, 12:15pm South Bank Busway.

    o Plan to catch an earlier bus if you wish to arrive a bit earlier, since Workshops begin at 13:00.

- City Cat Ferry from South Bank 2 Terminal (BCEC/South Bank Area) or North Quay 1 Terminal (City Centre); traveling to UQ St Lucia.

    o About 25 mins travel time, runs every 15 mins. This is the scenic route upstream along the river, which is highly recommended if you have time and leisure and want to let the river breeze blow the jet lag out of your brains.

    o City Cat to catch to be on time for the workshops: 12:06 pm South Bank 2 Terminal, 12:09 pm North Quay 1 Terminal.

It takes appx 10-15 minutes to walk on campus from the City Cat Ferry Stop/UQ Lakes Bus Station to the Sir James Foots Building. Please plan your journey to arrive at Sir James Foots Building by 12:45pm to ensure the workshops start on time. See the next page for directions to walk on campus.

Link to map illustrating transportation options is below.

    o Use routes on the left side to select your arrival plan.

    o https://www.google.com/maps/d/viewer?mid=1SoJi1FKVUsxZ6Jcmn9J5kHQEjXc&ll=-27.48451900067751%2C153.01653739999995&z=15

For more information on how to get to UQ, or how to use South East Queensland's public transport system please visit the Translink web page: www.translink.com.au

Lunch options nearby University of Queensland

Catering options on the UQ campus that are open for lunch on Sunday include:

Wordsmiths, Bar Merlo (at the Duhig Building), Burger Urge, and Saint Lucy's Caffe e Cucina.

For more information on finding these outlets and navigating the UQ Campus download the free "UQ Nav" and/or "UQ Walking Tour" apps to your mobile phone.

In addition, there is a plethora of food options available in the South Bank area near the BCEC if you want to have lunch before you head out to UQ. See Grey Street and Little Stanley Street appx 2 blocks from the BCEC.

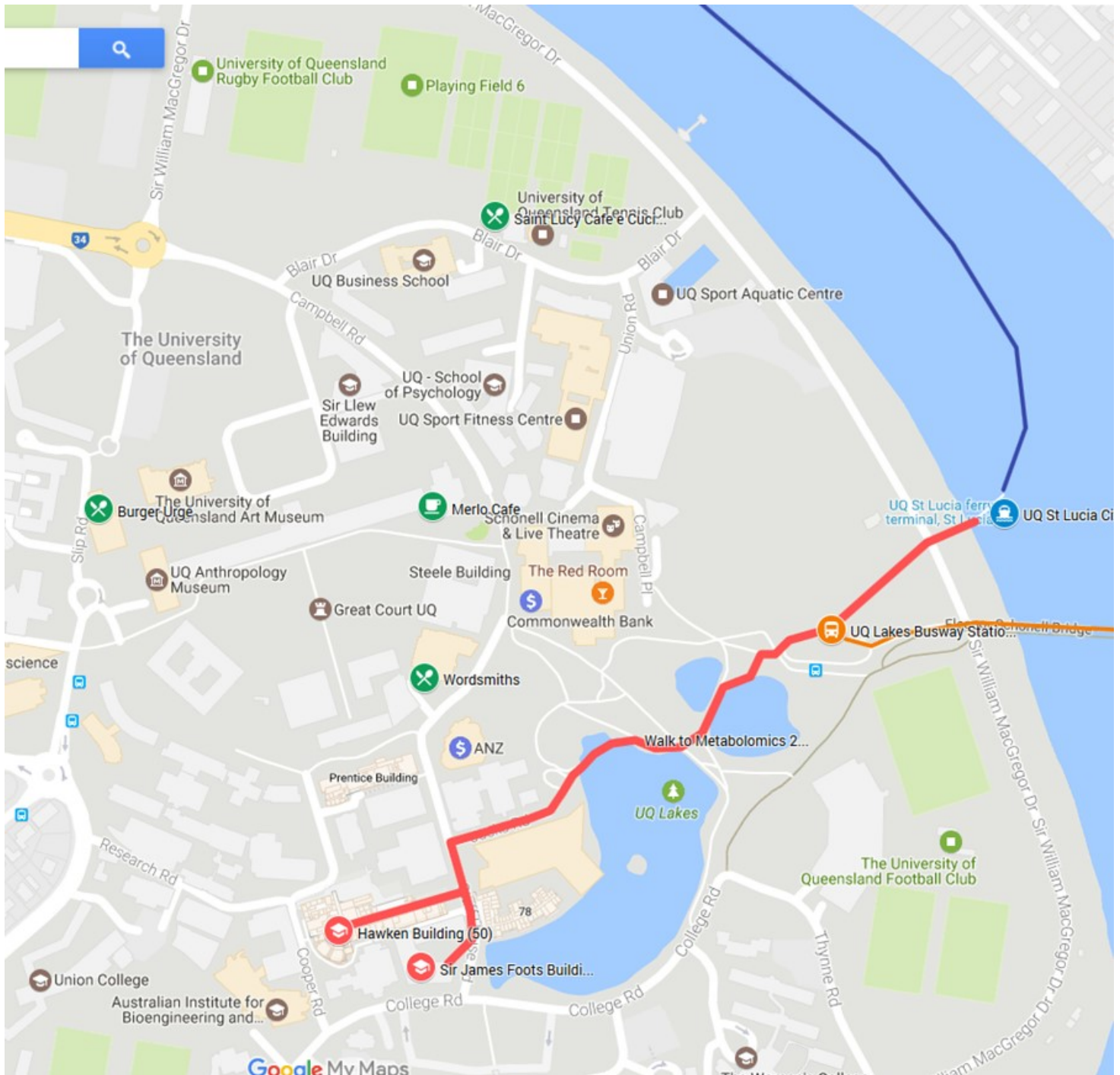# Workshops on Monday, June 26 take place at the BCEC.

Walking directions on campus to:

Sir James Foots Building:
MetaboTools - Room 47A-341
ANZMET Round Table - Room 47A-241
Network Medicine - Room 47A-241

Hawken Building:
EMN Workshops - Room 50-T203
(Raybould Lecture Theatre)

[Click here to view this map.](#)

WORKSHOP #1

MetaboTools: Analysis of metabolomics data in the context of the metabolic model

THEME: Building Bridges — Metabolic Modelling

LOCATION: University of Queensland St. Lucia

DATE AND TIME: Sunday 25 June 13:00–17:30 (Break 15:00–15:30)

ORGANIZERS: Dr. Maike K. Aurich, Luxembourg

ABSTRACT:
Constraint-based metabolic models consider in detail the metabolite transformations that appear in living cells at steady-state. They can be used to predict intracellular flux routes connecting metabolites cells consume to byproducts they release (exo-metabolome). MetaboTools provides extensive support for the analysis of extracellular metabolomic data in the context of the metabolic model. We will provide lectures at the beginning of the workshop to ensure a basic common understanding of the constraint-based modeling and analysis (COBRA) approach. Hands-on training of a computational workflow of data preparation, integration, and model analysis will allow the participants to get first-hand experience on the requirements, analysis possibilities, and the limits of the intra-model analysis of exo-metabolomic data using MetaboTools. The workshop is designed for participants with limited experience in metabolic modeling and programming.

OBJECTIVES:
- Get hands-on experience on the requirements, analysis possibilities, and the limits of the intra-model analysis of exo-metabolomic data using MetaboTools

LEARNING OUTCOMES:
- Basic understanding of the constraint-based metabolic modeling approach
- Basic understanding of data integration strategies and model analysis
- Gather first-hand experiences with the computational set-up

SCHEDULE

Time	Presenter	Topic
13:00–15:00	**Maike K. Aurich** *Research Associate, Luxembourg Centre for Systems Biomedicine, Luxembourg*	**Quick-starter lectures** Ensure a basic (common) understanding of the subject of the workshop and that the participants can reach the aim of the workshop. 1. Modeling approach and the metabolic model 2. Data integration strategies and model analysis
15:30–17:00	**Maike K. Aurich** *Research Associate, Luxembourg Centre for Systems Biomedicine, Luxembourg*	**Hands-on exercises** Guided tutorial through the complete workflow of data preparation, integration, and model analysis

WORKSHOP #2

ANZMET Round Table + Peer Sessions

THEME: Advancing the Field

LOCATION: University of Queensland St. Lucia

DATE AND TIME: Sunday 25 June 13:00-15:00

ORGANIZERS: Dr. Devin Benheim, La Trobe University; Dr. David de Souza, Metabolomics Australia; and Dr. Damien Callahan, Deakin University; The Australian & New Zealand Metabolomics Conference (ANZMET).

ABSTRACT:

The hallmark features of the ANZMET Conference (Australian & New Zealand Metabolomics Conference; www.anzmet.org) are its use of facilitated networking through the Round Table Discussion & Peer Sessions. These workshops expose delegates of Metabolomics2017 to a smaller version of the powerful and extremely well-received ANZMET flavor and format:

The roundtable discussion is designed to get the creativity flowing, gathering a rich stew of ideas, themes, desires and questions bubbling in people's minds! The roundtable provides an opportunity early in the conference to discover other attendees with similar interests and relevant experience. This session helps to determine the Peer Session topics.

The Peer Sessions are informal, topical, focused sessions facilitated by attendees which are interactive and friendly environments. They provide an engaging interpersonal process for open debate, discussion, answers to pressing questions and the development of ideas.

The peer sessions of ANZMET have resulted in the publication of several position papers in the journal metabolites.

We invite all delegates attending to participate in this years' publications: http://www.mdpi.com/journal/metabolites/special_issues/Metabolomics_Society.

This session is best experienced with a broad demographic of students, researchers, vendors and industry partners in attendance.

OBJECTIVES:
- Facilitated Networking during the Roundtable Discussion
- Topical and Focused Discussion in Peer Sessions

LEARNING OUTCOMES:
- Provides a rich and diverse environment for networking between all delegate demographics
- Allows for topical and engaging discussion in spontaneously selected topic(s) by attendees, culminating in one or more publications and/or position papers in the Journal Metabolites

SCHEDULE:

Time	Presenter	Topic
13:00–13:05	**Devin Benheim** *President, ANZMET Conference. Honorary Research Fellow, La Trobe University.*	Introduction
13:05–14:00	**Devin Benheim, David de Souza, Damien Callahan** *Roundtable Discussion & Nomination of Peer Session Topic(s)*	Facilitated Networking
14:00–15:00	**Devin Benheim, David de Souza, Damien Callahan** *Peer Sessions & Position Papers/Publications Signup*	Spontaneous Topic Selection

WORKSHOP #3

EMN Workshop — Experimental Design in Metabolomics: How to get started?

THEME: Advancing the Field

LOCATION: University of Queensland St. Lucia

DATE AND TIME: Sunday 25 June 13:00–15:00

ORGANIZERS: Tim Causon, University of Natural Resources and Life Sciences, Vienna, Austria (Moderator); Julia Kuligowski, Health Research Institute La Fe, Valencia, Spain; and Johannes Fahrmann, University of Texas MD Anderson, USA

ABSTRACT:

The application of metabolomics has become an important part of biological hypotheses generation and testing over the last 15 years. With a wide range of research questions now seeking metabolome-level information, it brings together a combination of biological, analytical, statistical, and computational elements entailing the use of multidisciplinary skill-sets. Hence, experimental design, including sampling considerations, choice of appropriate analytical strategies (platforms and methods), and quality control assessment play a key-role for a successful metabolomics study in order to allow robust datasets to be produced for meaningful statistical analysis and biological interpretation. This workshop will showcase

experts discussing the core goals of experimental design in metabolomics. Possible solutions for commonly encountered challenges in both planning metabolomics studies and selection of suitable analytical strategies including quantification and data quality considerations will also be addressed.

OBJECTIVES:

· The primary intent of this workshop will be focused on two principle aspects: study design considerations and experimental approach.

· Presentations from experts in the field will address education and training needs of researchers new to the field and with different scientific backgrounds including the use of case study examples to help develop core competencies in experimental design for metabolomics studies.

LEARNING OUTCOMES:

· Before you get started: Thoughts about the importance and challenges of the study design:

    · Sample size and statistical power

    · Sample collection, handling, and storage considerations

    · Potential bias and challenges.

· Analytical strategies: Does the method fit the purpose?

    · Choosing appropriate analytical platforms and methods

    · Quality control in measurement

    · Quantification approaches

SCHEDULE:

Time	Presenter	Topic
13:00–13:05	**Tim Causon** *Senior Scientist, University of Natural Resources and Life Sciences, Vienna, Austria*	Introduction
13:05–13:35	**David Broadhurst** *Professor, Edith Cowan University, Perth, Australia*	Before you get started: Thoughts about the importance and challenges of the study design
13:35–14:05	**Kati Hanhineva** *Adjunct Professor, Coordinator for LC-MS Metabolomics Center, University of Eastern Finland, Kuopio Area, Finland*	Choosing appropriate analytical platforms and methods
14:05–14:35	**Sastia Putri** *Assistant professor, Osaka University, Osaka, Japan*	Quantification approaches and Quality Control in measurement
14:35–14:55	**All speakers**	Open discussion and questions
14:55–15:00	**Tim Causon** *Senior Scientist, University of Natural Resources and Life Sciences, Vienna, Austria*	Closing remarks

WORKSHOP #4

Network medicine approaches for the analysis of metabolomic data

THEME: Metabolomics in Health and Medicine

LOCATION: University of Queensland St. Lucia

DATE AND TIME: Sunday 25 June 15:30–17:30

ORGANIZERS: Jessica Lasky-Su, Sc.D, Brigham and Womens Hospital Harvard Medical School

ABSTRACT:

Network medicine is a rapidly emerging field that integrates systems biology and network science in the study of complex disease. It provides a holistic approach to better understand disease through the identification and investigation of linear and nonlinear relationships and networks of interacting components. Network medicine and its underlying concepts have numerous applications in many different biological contexts for the study of disease etiology, diagnosis, phenotyping and treatment.

Network medicine is particularly well-suited to the study of metabolomics datasets. These high dimensional, highly collinear and noisy datasets pose a number of analytical challenges that have yet to be fully addressed. To date network approaches have not been widely used in the study of such data, yet the inherent structure and comprehensive nature of metabolomic networks means that these methods are ideal for maximizing the information that can be gleaned from metabolomic studies.

This workshop will provide an introduction to the concepts of network medicine, an overview of network approaches in the analysis of metabolomic data, a discussion of the utility of networks in integrative omics studies, an opportunity for network visualization and an exploration of the advantages and potential pitfalls of such approaches.

OBJECTIVES:

- To introduce the concepts and theories underlying network based approaches in systems biology

- To explore the utilities, advantages and potential pitfalls of network approaches in the study of metabolomic data

LEARNING OUTCOMES:

This workshop will provide attendees with the basic skills necessary to apply network approaches in their analysis of metabolomics data moving forward, specifically to:

- Understand the concept of network medicine and its role in the study of biology and disease

- Explore how metabolic pathways can be related to metabolomic networks

- Identify dynamic networks in large metabolomic profiling datasets, and distinguish the hubs, nodes and edges comprising these networks

- Recognize the limitations and potential pitfalls of these approaches, and consider how the continued development of the field is aiming to address these challenges

SCHEDULE:

Time	Presenter	Topic
15:30–16:30	**Jessica Lasky-Su, Sc.D (moderator)** *Associate Professor , Channing Division of Network Medicine, Brigham and Womens Hospital Harvard Medical School*	Network theory and the concepts of network medicine
16:30–17:30	**Rachel Kelly, PhD** *Postdoctoral Research Fellow , Channing Division of Network Medicine, Brigham and Womens Hospital Harvard Medical School*	The application of network medicine to metabolomics datasets

WORKSHOP #5

EMN Workshop — MS Metabolomics Data Processing

THEME: Metabolomics in Health and Medicine

LOCATION: University of Queensland St. Lucia

DATE AND TIME: Sunday 25 June 15:30–17:30

ORGANIZERS: Jan Stanstrup, Steno Diabetes Center, Denmark; and Charmion Cruickshank-Quinn, University of Colorado Anschutz Medical Campus, USA

ABSTRACT:
Processing large amounts of untargeted metabolomics data can be daunting, and the publicly available software tools rarely include an easy-to-understand walk-through. Participants will learn about several open source tools for analyzing their untargeted LC/MS and GC/MS data and how to get their spectra and raw data in the format needed for statistical analysis. The workshop will explain XCMS, CAMERA, and associated tools to process untargeted metabolomics data by providing examples, and demonstrating how to use the software. There will be a focus on practical skills and pitfalls so that the participants have an understanding of how to approach their data and answer their questions after the workshop.

OBJECTIVES:

- To teach participants how to import their data for use in XCMS
- To demonstrate how results can vary based on parameters
- To present databases for metabolite annotation with a focus on CAMERA in XCMS

LEARNING OUTCOMES:

- Participants will be able to process their own untargeted LC-MS and GC-MS metabolomics data
- Attendees will know how to use CAMERA to perform metabolite annotation
- Attendees will learn the appropriate normalization and imputation strategies

SCHEDULE:

Time	Presenter	Topic
15:30–16:10	**Jan Stanstrup** *Research Scientist, Steno Diabetes Center Copenhagen, Denmark*	LC/MS pre-processing: XCMS and parameter optimization
16:15–16:35	**Charmion Cruickshank-Quinn** *Instructor, University of Colorado Anschutz Medical Campus, USA*	Annotation: CAMERA and databases
16:40–17:10	**Warwick B. Dunn** *Senior Lecturer & Director of Mass Spectrometry, University of Birmingham, UK*	Comparison of strategies for normalization, missing value imputation, transformation and scaling
17:15–17:30	**Panel Discussion**	Discussion: Post data extraction

WORKSHOP #6

Hybrid Ion Mobility MS

THEME: Advancing the Field

LOCATION: BCEC

DATE AND TIME: Monday 26 June 8:45–10:15

ORGANIZERS: Endre Laczko, Head Metabolomics Group at FGCZ, ETH Zürich and University of Zürich, Switzerland (Moderator)

ABSTRACT:

Hybrid Ion Mobility — Mass Spectrometry systems (IMS – MS) are known for many years. Today, IMS-MS systems are available from several vendors (TofWerk, Waters, Agilent, Bruker, ABSciex, Thermo may follow soon), however they are still rarely used for metabolomics. In this workshop the currently available IMS-MS types will be presented and their use for metabolomics will be discussed. Further, it will be explained how an IMS-MS method is set up and how the resulting data is analysed. Exemplary cases will allow the participants to valuate IMS-MS metabolomics data in comparison to metabolomics data from other systems currently in use. It is planned to include a Q&A session and to explore the interest for an IMS user group.

OBJECTIVES:

- Presenting applications of ion mobility – MS in metabolomics studies
- Highlighting advantages of ion mobility – MS
- Initiating an interest group Ion Mobility – MS under the umbrella of the International metabolomics Society

LEARNING OUTCOMES:

- Valuation of the use of ion mobility – MS
- Basic knowledge to set up a workflow based on ion mobility – MS
- Knowing people already using ion mobility – MS in metabolomics, including lipidomics

SCHEDULE:

Time	Presenter	Topic
8:45–9:00	**Endre Laczko** *Head Metabolomics Group at FGCZ, ETH Zürich and University of Zürich, Switzerland*	Introduction
9:00–9:20	**Endre Laczko** *Head Metabolomics Group at FGCZ, ETH Zürich and University of Zürich, Switzerland*	A protocol for human blood analysis
9:20–9:40	**Tim Causon** *Senior Scientist, BOKU Vienna, Austria*	Drift tube ion mobility-mass spectrometry for metabolomics
9:40–10:00	**All presenters**	Q&A
10:00–10:15	**All presenters**	Interest Group IMS-MS

WORKSHOP #7

Role of Metabolomics for Health & Diet Research

THEME: Metabolomics in Health and Medicine

LOCATION: BCEC

DATE AND TIME: Monday 26 June 8:45–10:15

ORGANIZERS: Lee Gethings; Antonietta Wallace; and David Heywood (Moderator), Waters Corporation

ABSTRACT:
Application of OMIC workflows, particularly metabolomics has shown to provide insight into health and food as well as the complex relationship which exists between both. Understanding bioavailability of food in the body for short and long term wellbeing is of increasing interest. New research is emerging based on advances from technology and metabolomic standpoints, to understand the nature of disease, nutritional diet and the role diet plays physiologically.

This interactive workshop will provide in-depth discussion regarding technological advances from an LC-MS, ambient ionisation and informatic perspective. Integration of these technologies into metabolomic workflows will be presented by leading academic and industrial users, demonstrating how these approaches can be used to better understand the complex relationship between diet and health.

OBJECTIVES:
- Review new analytical approaches and workflows being successfully applied to understanding the role of metabolomics in food and health research
- Discuss the challenges associated with Metabolomics in complex matrices and how new technological advancements are addressing these challenges

LEARNING OUTCOMES:
- Relate methodologies used in metabolomics and food research to specific analytical challenges
- Be able to understand where new technologies can benefit metabolomics applications
- Appreciate the relationship between biological systems, disease, environment and food

SCHEDULE:

Time	Presenter	Topic
8:45–9:05	**Prof. Stephen Blanksby** *Director, Central Analytical Research, Queensland University of Technology, Australia*	High-pressure Ozone-Induced Dissociation for Lipid Structure Elucidation on Fast Chromatographic Timescales
9:05–9:15	**Dr. Paul Goulding** *Business Development Manager, Nonlinear Dynamics, UK*	An Enhanced Discovery 'Omics Workflow in Complex Biological Matrices
9:15–9:35	**Dr. Marten Snel** *Principal Research Fellow, SAHMRI, Australia*	Are identical mice the same? The gut microbiome and faecal metabolome in mouse models
9:35–9:55	**Dr. Fe Calingacion** *Postdoctoral Research Fellow, University of Queensland, Australia*	A multi-omics approach to understand grain quality using a diverse set of rice
9:55–10:05	**Dr. Sarah Stead** *Principle Scientist MS Technologies, Waters Corporation, UK*	Rapid Evaporative Ion Mass Spectrometry: An emerging disruptive technology for foodomics
10:05–10:15	Discussion	

WORKSHOP #8

Data Sharing, Standardisation and Workflow for reproducible analysis in Metabolomics

THEME: Advancing the Field

LOCATION: BCEC

DATE AND TIME: Monday 26 June 8:45–10:15

ORGANIZERS: Reza Salek (Chair/Moderator); Oliver Jones; Saravanan Dayalan; Masanori Arita; Pablo Moreno; and Christoph Steinbeck

ABSTRACT:
Reproducing results in any science is quite challenging. In the field of metabolomics, for results to become reproducible, descriptions of an investigation in a manuscript are not sufficient. To surpass this, and increase the chance of result reproducibility, standard frameworks for data sharing and sharing of experimental data are invaluable. We now have several data sharing platforms such as MetaboLights and Metabolomics Workbench that aim to make use of such standards to promote data-sharing. In this workshop, we will discuss data sharing as well as metabolomics data formats, much of which are adopted from the efforts in the proteomics HUPO-PSI initiative. Examples and application of data formats such as mzML and nmrML would be given. We will also present and discuss mzTab developments for metabolite identification. We will also demonstrate how emerging metabolomics data sharing platforms can promote open, accessible data sharing standards. Finally, we will discuss computational workflows for metabolomics data analysis within the PhenoMeNal e-infrastructure. We hope to make the metabolomics community aware of such efforts and ideally how to get involved.

OBJECTIVES:
- Overview of data standards formats
- Capturing and reporting meta-data
- Using workflow and PhenoMeNal compute infrastructure
- Reference spectra data exchange and remix

LEARNING OUTCOMES:
- Learning about different data standards efforts
- Importance of data sharing and Meta-data reporting
- Role of workflow and infrastructures for metabolomics data analysis
- Access and sharing reference spectra

SCHEDULE:

Time	Presenter	Topic
8:45–9:05	**Reza Salek** *EMBL-EBI, UK*	Data standards, data sharing and workflows in metabolomics — an overview
9:05–9:20	**Saravanan Dayalan** *University of Melbourne, AU*	Complying with international data standards through data management software
9:20–9:40	**Masanori Arita** *National Institute of Genetics, Japan*	Complying with standards in a multi-user environment: the case of MassBank
9:40–10:00	**Pablo Moreno** *EMBL-EBI, UK*	PhenoMeNal technical overview and how to bring your tools to the framework
10:00–10:15		Discussion and questions

WORKSHOP #9

EMN Workshop — Statistical Considerations and Pathway Analysis Strategies for Metabolomics Datasets

THEME: Building Bridges — Metabolic Modelling

LOCATION: BCEC

DATE AND TIME: Monday 26 June 8:45–10:15

ORGANIZERS: Johannes F. Fahrmann, University of Texas, MD Anderson, USA; Fidele Tugizimana, University of Johannesburg, South Africa; and Stacey Reinke, Murdoch University, Australia (Moderator)

ABSTRACT:

Over the past decade, major advancements in untargeted and targeted metabolomics technologies have enabled high-throughput analysis of 1000s of biochemical perturbations associated with various organismal processes and pathological conditions. Statistical analysis of large datasets remains a bottleneck. Furthermore, the successful integration and interpretation of metabolomic datasets requires adequate background knowledge of associated biochemical pathways, an aspect that may not be attributed to all scientists, particularly those that are new to the field. The primary intents of this workshop are to 1) highlight important statistical/chemometric considerations for metabolomic datasets and 2) provide education on biochemical pathway mapping approaches. This workshop is primarily targeted towards beginners in the metabolomics field, including early-career researchers, but also everyone who is using metabolomics to complement their own existing research.

OBJECTIVES:

- Statistical/chemometric considerations for metabolomic datasets

- Biochemical pathway mapping approaches

LEARNING OUTCOMES:

- Univariate and Multivariate Analyses for Metabolomic Datasets

- Statistical (Chemometric) Model (cross) Validation and Variable Selection

- Data Integration and Visualization — Pathway mapping

SCHEDULE:

Time	Presenter	Topic
8:45–8:50	**Fidele Tugizimana / Stacey Reinke** *EMN Committee* *University of Johannesburg, South Africa /* *Murdoch University, Australia*	Introduction
8:50–9:15	**Saravanan Dayalan** *Lead Scientist/ Bioinformatician, University of Melbourne, Australia*	Statistical/ chemometric considerations for metabolomic datasets
19:15–10:00	**Jianguo Xia** **Jourdan Fabien** *Assistant Professor, McGill University, Canada* *INRA UMR1331 Toxalim, France*	Biochemical pathway mapping approaches
10:00–10:15	**All presenters**	Q/A

Advances in High Throughput Targeted Metabolomics Analysis

THEME: Advancing the Field

LOCATION: BCEC

DATE AND TIME: Monday 26 June 10:30–12:00

ORGANIZERS: Alex Apffel, Agilent Laboratories; and Judith Denery, Amyris, Inc.

ABSTRACT:

In the last several years a number of approaches have been developed to increase the throughput of targeted metabolomics analysis. Each has advantages and disadvantages in terms of speed, sensitivity and specificity. Each has also been developed in a specific application context and designed to meet the needs of that application. This workshop will explore a number of these approaches while explaining how the technology serves the needs of the specific application area.

OBJECTIVES:

- Present needs of High Throughput (HTP) metabolomics, especially in the field of synthetic biology.

- Present several different approaches to HTP metabolomics

- Discuss limitations and opportunities for HTP metabolomics

LEARNING OUTCOMES:

- Develop familiarity with several different approaches to HTP mass spectrometric techniques for metabolomics

- Understand several applications for HTP metabolomics.

- Contribute and learn from discussion of strengths and limitations of current approaches to targeted HTP metabolomics.

SCHEDULE:

Time	Presenter	Topic
10:30–10:50	**Judith Denery** *Senior Scientist, BioAnalytics, Amyris, Inc., USA*	Introduction and Context for High Throughput Metabolomics
10:50–11:10	**Rich Ellson** *CTO and Co-Founder, Labcyte, Inc., USA*	Ultra-High Throughput Screening (UHTS) with Acoustic Mist Injection (AMI) Exceeds 100K Samples Per Day: Emerging Opportunities for Lipidomics and Metabolomics
11:10–11:30	**Steven Gross** *Professor of Pharmacology, Pharmacology, Weill Cornell Medical College, USA*	Multiplexed High-throughput Biomolecule Quantification Using RapidFire Mass Spectrometry
11:30–11:50	**Alex Apffel** Senior Research Scientist, Agilent Research Laboratories, USA	UHPLC-MS Approaches for High Throughput Metabolomics
11:50–12:00	**All**	Discussion

WORKSHOP #11

EMN Workshop — Career Development

WORKSHOP LOCATION: BCEC

DATE AND TIME: Monday 26 June 10:30–12:00

ORGANIZERS: Jan Stanstrup, Steno Diabetes Center Copenhagen, Denmark (Moderator); Stacey Reinke, Murdoch University (Moderator); and Fidele Tugizimana, University of Johannesburg

ABSTRACT:

Regardless of individual area of research, one topic that is invariably on the minds of all early-career researchers is their career. Many postgraduate degrees are not associated with clear career trajectories. Moreover, as students and postdocs are largely trained in the academic setting they lack exposure and training specific to other career paths. In this workshop, early-career researchers will hear from speakers who chose careers outside research-based academic positions. The speakers will use their own experience to formulate actionable career progression advice for early-career scientists. Following the presentations, we will have 30 minutes for open discussion and questions so that attendees can directly interact with our speakers. Through this workshop, we hope to make early-career researchers more aware of their career options and potential paths to obtain them.

OBJECTIVES:

- Improve awareness of career options for early-career researchers
- Help early-career researchers identify pathways and mechanisms to achieve these careers

LEARNING OUTCOMES:

- Appreciation that Academic Research is not the only career path.
- Recognition of the diverse careers available for a PhD scientist.
- Understanding what employers are looking for in early career scientists.
- Being able to weigh the pros and cons of the career paths discussed.

SCHEDULE:

Time	Presenter	Topic
10:30–10:50	**Krista Zanetti** *Program Director, National Cancer Institute, USA*	Career Pathways in Government
10:50–11:10	**Ralf Tautenhahn** *Product Manager Metabolomics Software, Thermo Fisher Scientific, USA*	Career Pathways for Industry
11:10–11:30	**Mary Boyce** *Associate Professor, Edith Cowan University, Australia*	Career Pathways for Academic Lecturers
11:30–12:00	**All**	Open discussion and questions

WORKSHOP #12

Metabolite Identification: Current Approaches and Reporting Standards

THEME: Building Bridges — Natural Products/ Metabolite Identification

LOCATION: BCEC

DATE AND TIME: Monday 26 June 10:30–12:00

ORGANIZERS: Dr Warwick Dunn, University of Birmingham, UK

ABSTRACT:

Metabolite identification (sometimes defined as annotation) is a key component of any untargeted metabolomics workflow to enable the delivery of biological knowledge and impact from analytical data. The processes applied to identify metabolites are numerous and are dependent on the complexity of sample, analytical platform applied and quality of data acquired. Based on the reported spectral evidence, a confidence level for the metabolite or feature identification is given. The development of reporting standards and in particular of confidence levels for metabolite identification was initiated in 2007 by the Metabolomics Standards Initiative [Sumner et al. Metabolomics, 2007, 3, 211] and these reporting standards are currently being assessed and revised. In this workshop a panel of experts will provide their current insights into the complexities and solutions for metabolite identification applying NMR spectroscopy, gas/liquid chromatography-mass spectrometry and imaging mass spectrometry, followed by a Q&A session to allow the metabolomics community to question the panel and also to provide their own insights and comments.

OBJECTIVES:
- To discuss the importance of reporting standards for metabolite identification and to gain additional insights from the community
- To discuss with the metabolomics community the multiple options applied to identify metabolites in metabolomics studies and to gain additional insights from the community

LEARNING OUTCOMES:
- Enhanced understanding of how to apply current and revised reporting standards for metabolite identification
- Enhanced understanding of how different technologies including NMR spectroscopy and hyphenated mass spectrometry can be applied for identification of metabolites in metabolomics studies
- To gain additional insights into preferred methods of metabolite identification confidence from the broader metabolomics community

SCHEDULE:

Time	Presenter	Topic
10:30–11:00	**Dr Warwick Dunn and Prof. Lloyd Sumner** *University of Birmingham, UK and University of Missouri, USA*	Introduction and reporting standards for metabolite identification
11:00–11.15	**Prof. Jules Griffin and Dr Neil Taylor** *University of Cambridge, UK and President, Chenomx Inc*	NMR and metabolite identification
11:15–11:30	**Prof. Robert Trengrove and Dr Darren Creek** *Murdoch University, Australia and Monash University, Australia and*	LC-MS, GC-MS and metabolite identification
11:30–11:45	**Dr Berin Boughton** *Metabolomics Australia, School of BioSciences, The University of Melbourne*	Mass spectral imaging and metabolite identification
11:45–12:00	**Members of the Metabolomics Society Metabolite Identification task group**	Ask the Experts session

WORKSHOP #13

WORKSHOP TITLE: Clinical Biomarker Detection

THEME: Metabolomics in Health and Medicine

LOCATION: BCEC

DATE AND TIME: Monday 26 June 10:30–12:00

ORGANIZERS: Dr Nicholas J W Rattray, Prof Roy Goodacre (Moderator)

ABSTRACT:

The development of metabolomics as a translational tool within the clinical realm is one of the major applications for our area of science, with important advances being made in areas such as risk

assessment, early detection and diagnosis of disease, prognosis of drug action and therapeutic evaluation. But the journey from biomarker discovery to clinical translation is a long one and requires an expert understanding and application of study design, sample prep and bioanalysis coupled with a functional understanding of the data that is generated. This inherent multi-levelled complexity is a major challenge in the field.

The purpose of this workshop is to overview the experimental workflow used within the biomarker development pipeline and will include insights from experts in the field of metabolomics who will give examples of their experiences and provide tips and advice to new-comers in the field and help explain how to overcome the issues of complexity. The overall aim is to showcase advances made in aspects such as design of experiments and interpretation of metabolite data in a clinical context and will thus align with the Health and Wellness focus of the conference.

OBJECTIVES:

- Highlight the history of the clinical biomarker development pipeline

- Discuss where future trends in technology and statistics may take the area

LEARNING OUTCOMES:

- Appreciation of the multidisciplinary nature of clinical biomarker detection

- Highlight issues of complexity within data and how to overcome them

- Understand how progress data quality has been underpinned by advances in instrumentation

SCHEDULE:

Time	Presenter	Topic
10:30–10:35	**Roy Goodacre** *Chair in Biological Chemistry University of Manchester (UK)*	Introduction
10:35–10:55	**David Broadhurst** *Chair in Data Science & Biostatistics, Edith Cowan University (AUS)*	Design of Experiments in Clinical Metabolic Profiling
10:55–11:15	**Nicholas Rattray** *Postdoctoral Research Associate, Yale School of Public Health, Yale University (USA)*	Technological Advancements Underpinning Metabolomics Growth
11:15–11:35	**Kevin Huynh** *PhD Student, Baker IDI Heart and Diabetes Institute (AUS)*	Clinical Translation with Large Cohort Studies
11:35–12:00	**Open Panel**	Discussion and Questions