

Workshop Program

Workshop Program Morning Sunday 27th Parallel session 1A:

	Topic	Coordinators
10.00 – 12.30	Mass Spectrometry: identification and quantification strategies This workshop aims to give an overview of MS-based techniques used in metabolomics research. Furthermore, we will discuss and review current trends in quantifying the right metabolites as well as strategies to identify (novel) metabolites using accepted protocols and novel methodologies. The workshop will address issues, like GC-MS and LC-MS, Quantification and ion suppression, various ionization techniques, why sample preparation?, multi-dimensional chromatography and mass spectrometry, metabolite identification from complex metabolomics data, etc. The workshop will supply you with the necessary knowledge to fully indulge in the programme of the conference and to get the best insight in the latest trends, techniques, challenges but also possibilities at hand nowadays.	Rick Dunn (UK) & Rob Vreeken (Netherlands)
10.05 – 10.35	Introduction to the application of Mass Spectrometry in Metabolomics Ute Roessner (Australia)	
10.35 – 10.55	Biomarker and profiling strategies for the diagnosis of Tuberculosis using GC and GC X GC-Tof-MS. Erwin Kaal (Netherlands) (Sponsored by LECO)	
10.55 – 11.20	Latest trends in getting accurate Metabolite concentrations in metabolomics studies Rob Vreeken (Netherlands)	
11.20 – 11.45	Identification of metabolites: Current Techniques and Novel Approaches Warwick (Rick) Dunn (UK)	
11.45 – 12.05	Technology Spotlight: Latest developments in High definition Mass Spectrometry(HDMS). Presented by John Rontree (Sponsored by Waters)	
12.05 - 12.30	Open discussion forum Lead by Rob Vreeken and Rick Dunn.	

Workshop Program Morning Sunday 27th Parallel session 1B:

	Topic	Coordinators
10.00 – 12.30	<p>NMR spectroscopy: What's new?</p> <p>To date these workshops have focused on teaching various aspects of NMR spectroscopy. This year, we have decided to break from this format and instead tried to show the full range of what NMR spectroscopy has to offer. While all talks will be geared to educate, new results and techniques will be presented to show how NMR spectroscopy is used in solution state and solid state, in vitro and in vivo, and in both steady state and in dynamic experiments.</p>	Jules Griffin (UK & Aalim Weljie (Canada)
10.00 – 10.30	<p>A journey from in vivo NMR to metabolomics: from MRS to OPLS. Hans Vogel (Calgary, Canada)</p>	
10.30 – 10.55	<p>HR-MAS proton NMR based metabolomic analysis of breast cancer tissues highlight the importance of choline metabolites in tumour grading. Reza Salek (Cambridge, UK)</p>	
10.55-11.20	<p>Metabolic Profiling Detects Systemic Effects of Environmental and Lifestyle Exposure to Cadmium in a Human Population. James Ellis (London, UK)</p>	
11.20-11.45	<p>Investigating the Metabolic Effects of Heart Failure Progression using Hyperpolarized Magnetic Resonance Helen Atherton (Oxford, UK)</p>	
11.45-12.10	<p>Novel Methods for Identifying and Quantifying Metabolites in Complex Biological Extracts by Multidimensional Nuclear Magnetic Resonance Spectroscopy Ian Lewis (Princeton, USA)</p>	
12.10 - 12.30	<p>Don't put my peaks in a bucket – alternative ways for data processing of NMR spectra + Discussion. Julian Griffin (Cambridge, UK) & Aalim Weljie (Calgary, Canada)</p>	

Workshop Program Afternoon Sunday 27th: Parallel session 2A

	Topic	Coordinators
	<p>Biostatistics, chemometrics and bioinformatics The goal of the biostatistics workshop is to review a large part of the data analysis pipeline. Study design as well as measurement design, thus <i>which samples are taken when?</i> and <i>when are they measured?</i> are important questions we aim to answer. Furthermore the whole data laundry process to clean up the “dirty data” will be reviewed. We will look into the use of databases during the data analysis process and finally the data analysis of designed studies and its validation receives sufficient attention.</p>	Johan Westerhuis (Netherlands) & Roy Goodacre (UK)
14.00 – 14.25	<p>Measurement design and corrections in metabolomics. Adrie D. Dane (Netherlands)</p>	
14.25 – 14.50	<p>Use of web-based databases and applications for quantitative metabolomic studies. Jianguo (Jeff) Xia (Canada)</p>	
14.50 – 15.15	<p>Analyzing structured metabolomics data. Age K. Smilde (Netherlands)</p>	
15.15 – 15.40	<p>Processing of mass spectrometry based molecular profile data Matej Orešič (Finland)</p>	
15.40 – 16.05	<p>Validation and biomarker selection in metabolomics data analysis Johan A. Westerhuis (Netherlands)</p>	
16.05 – 16.30	<p>General Discussion on future initiatives Lead by Roy Goodacre and Johan Westerhuis</p>	

Workshop Program Afternoon Sunday 27th: Parallel session 2B

	Topic	Coordinators
	<p>Plant metabolomics In the plant metabolomics workshop the potentials and pitfalls of the main technologies available for wet lab analyses will be covered. Starting with the importance of experimental design and sampling approaches, aspects data acquisition and processing will be covered as will opportunities for automation of procedures for large sample numbers. This will be followed by a 'Research blast' where 6 scientists with the most innovative poster abstracts will each have 5 minutes to present their work. A general discussion of future developments will round off the workshop.</p>	Lloyd Sumner & Robert Hall
14.00 – 15.00	<p>Plant Metabolomics technology review. Mike Beale & Jane Ward (UK)</p>	
15.00 – 15.45	<p>Research Blast 6 x 7 minute poster shots!</p> <ul style="list-style-type: none"> ➤ ➤ ➤ ➤ ➤ ➤ 	Choices now being made!
15.30 – 16.30	<p>Open discussion on future developments, opportunities for collaborative efforts, future meetings etc Lloyd Sumner & Robert Hall</p>	

Additional Workshop Program Monday 28th Parallel Session 3A:

	Topic	Coordinators
18.30 – 19.45	Databases & Standards Discussion session In this session a number of key points will be brought to the table for discussion and exchange of ideas and experiences. Important here are for example, topics related to ease of accessibility and reliability of (unpublished) datasets and how we can ensure that these are robust and usable to others. Robustness also relies upon correct unambiguous annotation – what are your experiences? The general aim therefore is to exchange ideas and if possible come to a consensus on at least some of these issues and / or to establish a means to continue discussions in order to solve some of these issues.	Oliver Fiehn & Christoph Steinbeck
18.30 – 19.30	(1) Publications: how can we improve the public accessibility of metabolomic data sets? (2) Existing databases: how can we improve usability of databases from MassBank to MetaCyc and ChEBI? What are the sets of data that users would like to get from databases but that are not yet available? (3) Metabolite queries: How do we make sure we talk about the same compounds when using queries? How do we correct wrong entries in databases? (4) Quantifications: How do we deal with the problem that absolute quantifications are inherently difficult but relative normalizations are not comparable between studies? Are they?	
19.30 – 19.45	(5) Round –up discussion: How and where can we collect ideas, links and comments in a Wiki- or Blog-style to continue discussions?	

Additional Workshop Program Monday 28th Parallel Session 3B:

	Topic	Coordinators
18.30 – 19.45	Nordic Interest Group	Matej Oresic
18.30 – 19.00	Introduction of metabolomics research activities in Nordic countries Group presentations from Denmark, Finland, Norway, Sweden	
19.00 – 19.45	General discussion and Organization issues: Conferences, workshops, training etc Lead by Matej Oresic	

Additional Workshop Program Tuesday 29th Parallel Session 4A:

	Topic	Coordinators
18.30 – 19.45	<p>Environmental metabolomics</p> <p>The environmental metabolomics session has been organised to cover key issues of wide relevance to the community. The workshop has been divided into 4 main topics which will be introduced by a leading scientists which will then be followed by a open floor discussion for input from anyone involved. The main aim is to exchange information (<i>who is doing what? Using which organism? Which systems? Which technical and biological limitations are being experienced? etc</i>) and discuss ideas and establish an interactive forum for future collaboration, organisation of workshops / meetings etc.</p>	Mark Viant & Dan Bearden
18.30 – 18.45	<p>Discussion Topic 1 – International NMR intercomparison exercise</p> <p>Lead: Dr Dan Bearden, NIST</p>	
18.45 – 19.00	<p>Discussion Topic 2 – Metabolomics in environmental/ecological risk assessment</p> <p>Lead: Dr Mark Viant, University of Birmingham</p>	
19.00 – 19.15	<p>Discussion Topic 3 – Brainstorming on “what are the top 5 or 10 measurement problems in environmental metabolomics?”</p> <p>Lead: Dr Dan Bearden (USA)</p>	
19.15 – 19.30	<p>Discussion Topic 4 – What is the purpose of environmental metabolomics?</p> <p>Lead: Dr Jake Bundy (UK)</p>	
19.30 – 19.45	<p>Round up summary</p>	

Additional Workshop Program Tuesday 29th Parallel Session 4B:

	Topic	Coordinators
18.30 – 19.45	<p>Pharma & Future of Health System</p> <p>The aim of this session is to address key issues in the area of the application of metabolomics in health care, daily clinical decisions and in the pharmaceutical industry.</p> <p>The following topics will be addressed by leading scientists from academia, clinical experts and patient organizations followed by a round table discussion</p> <ul style="list-style-type: none"> • What is necessary to make metabolomics a routine tool in clinical decision making? • What are lessons to be learned from other omics? • How can metabolomics change the current practice in health care and in the pharmaceutical industry? 	Thomas Hankemeier & Rima Kaddurah - Daouk
18.30 -	Programme will follow soon	