

# Mass Spectrometry and Proteomics Congress 2016

Developments in Mass Spectrometry and Proteomics for Progressing Medical Research

Global Engage are pleased to announce the inaugural Mass Spectrometry and Proteomics Congress, which will be held on 14th-15th November 2016 in London. The event is part of our highly successful series of life science technology congresses including conferences on Microfluidics, qPCR and Digital PCR, and Precision Medicine amongst others.

Attracting experts working in all areas of mass spectrometry, including MALDI-TOF, ionisation techniques, MS imaging, sample preparation, high-throughput techniques and data interpretation, the conference will examine the latest developments in the technologies and methods being used for progressing medical research in areas such as disease diagnostics, metabolomics, proteomics, drug discovery, virology and genomics. The challenges and possibilities of mass spectrometry will also be examined.

Mass spectrometry is an analytic technique with an increasing presence in both laboratory and clinical research, and scientists are continually discovering the wide range of possibilities the technology can provide. As mass spectrometry techniques become ever more invaluable to areas of research such as proteomics and diagnoses, the field is receiving growing attention as a tool for progressing medical studies. Indeed, it is estimated that the global market for this technology will reach \$5.9 billion by 2018.

The conference will provide an interactive networking forum to both further develop and answer your queries through a vibrant exhibition room full of technology providers showcasing their technologies and other solutions, poster presentation sessions, expert led case study presentations and interactive Q&A discussions from a 40-strong speaker faculty examining topics on 3 separate tracks outlined below.

## Confirmed Speakers Include:



**Alan Marshall**  
Professor of Chemistry and Biochemistry, Florida State University and Chief Scientist, Ion Cyclotron Resonance Program, National High Magnetic Field Laboratory, USA



**Carol Robinson**  
Dr. Lee's Professor of Chemistry, University of Oxford, UK



**Ron Heeren**  
Limburg Chair, Professor of Molecular Imaging and Director of M4I (the Maastricht MultiModal Molecular Imaging Institute), Maastricht University, The Netherlands

## Conference Synopsis

### Day 1 – Stream One

#### Mass Spectrometry: Strategies and Technologies

- Comparing MS methods e.g.
  - Quadrupole MS, Tandem MS, LC-MS and GC-MS, ICP-MS, IMS, MALDI-TOF, SIMS, AMS, TIMS, CE-MS
- New Developments in MS Instruments
- Sample Preparation
- Ionisation Techniques
- Standardisation, Validation, and Regulation
- Automation and Liquid Handling
- System Configuration
- Ultrahigh-Resolution and Ultra-Sensitive MS
- Mass Spectrometry Imaging Developments
- Assay Development for Clinical Applications

### Day 2 – Stream One

#### Mass Spectrometry Related Methodologies

- Developments in Separation Science
- Chromatography Improvements
- High-Throughput Techniques
- Top-down vs Bottom-up Proteomics
- Peptide Mapping
- Proteomics Workflow Optimisation
- Data Analysis and Databases
- Bioinformatics
- Computational Analysis and Software Solutions

### Day 1 and 2 – Stream Two

#### Healthcare Case Studies and Applications

- Clinical Applications of Mass Spectrometry and Proteomics
- Drug Discovery and Development
- Biomarker Detection and Diagnostics
- Screening Assays
- Proteomics
  - Precision Proteomics and Personalised Medicine
  - Protein Identification and Structural Elucidation
  - Protein-Protein Interaction Quantification
  - Glycan Analysis
- Pharmacokinetics and Pharmacodynamics
- Metabolomics including Lipidomics
- Case studies also looking into:
  - Small Molecule Analysis
  - Oncology
  - Virology/Bacteriology
  - Toxicology
  - Histology
  - Microbiology

# Mass Spectrometry and Proteomics Congress – 14-15 November 2016, London, UK

## Confirmed Speakers



**Alan Marshall**  
Professor of Chemistry and Biochemistry, Florida State University and Chief Scientist, Ion Cyclotron Resonance Program, National High Magnetic Field Laboratory, USA



**Carol Robinson**  
Dr. Lee's Professor of Chemistry, University of Oxford, UK



**Jonathan Wingfield**  
Principal Scientist, AstraZeneca, UK



**Christian Janfelt**  
Associate Professor and PI of the Mass Spectrometry Imaging Laboratory, University of Copenhagen, Denmark



**Loïc Dayon**  
Proteomics Team Leader, Nestlé Institute of Health Sciences, Switzerland



**Frank Vanhaecke**  
Professor of Analytical Chemistry, Ghent University, Belgium



**Carsten Hopf**  
Professor and Head of the Research Center for Applied Biomedical Mass Spectrometry (ABIMAS), Mannheim University of Applied Sciences, Germany



**Peter James**  
Professor of Protein Technologies, Lund University, Sweden



**Claire Evers**  
Professor of Biological Mass Spectrometry, University of Liverpool, UK



**Frank Sobott**  
Professor of Biomolecular and Analytical Mass Spectrometry, University of Antwerp, Belgium



**Simone Nicolardi**  
Senior Researcher, Leiden University Medical Center, The Netherlands



**Rene Zahedi**  
Group leader in Protein Dynamics, ISAS Institute, Germany



**Simon Hubbard (Track Chair)**  
Professor of Computational Biology, University of Manchester, UK



**Jennie Lill**  
Director, Proteomics and Biological Resources, Genentech, USA



**Jonathan Blackburn**  
Research Chair, Applied Proteomics and Chemical Biology, University of Cape Town, South Africa



**Sara Lind**  
Associate Professor, Uppsala University, Sweden



**Benedikt Kessler**  
Professor of Biochemistry and Life Science Mass Spectrometry, University of Oxford, UK



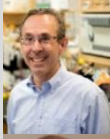
**Juan Antonio Vizcaino**  
Proteomics Team Leader, EMBL-European Bioinformatics Institute, UK



**Julia Chamot-Rooke**  
Head of Structural Mass Spectrometry, Institut Pasteur, France



**Richard Scheltema**  
Junior Assistant Professor, University of Utrecht, The Netherlands



**David Litchfield**  
Professor of Biochemistry and Oncology, Chair of Biochemistry, University of Western Ontario, Canada



**Georgios Theodoridis**  
Professor of Chemistry, Aristotle University Thessaloniki, Greece



**Helen Cooper**  
Professor of Mass Spectrometry, University of Birmingham, UK



**Tao Liu**  
Senior Staff Scientist, Pacific Northwestern National Laboratories, USA



**Steven Olde-Damink**  
Professor of Surgery and Director of Research, Maastricht University, The Netherlands



**Konstantinos Thalassinou**  
Senior Lecturer in Biophysical Mass Spectrometry, University College London, UK



**Ron Heeren**  
Limburg Chair, Professor of Molecular Imaging and Director of M4I (the Maastricht MultiModal Molecular Imaging Institute), Maastricht University, The Netherlands



**Michelle Hill**  
Associate Professor and Head of the Cancer Proteomics Group, University of Queensland Diamantina Institute, Australia



**Filip Cuyckens**  
Scientific Director & Fellow, Pharmacokinetics, Dynamics & Metabolism, Janssen R&D, Belgium



**Tony Whetton**  
Director, Stoller Biomarker Discovery Centre and Director, Manchester Precision Medicine Institute, UK



**Peter Lasch**  
Group Leader, Robert Koch Institute, Germany



**Joerg Hoenschemeyer**  
Head of Mass Spectrometry Laboratory for Peptides, Oligonucleotides and Proteins, Preclinical CMC, Roche Innovation Centre, Basel, Switzerland



**Christopher Gerner**  
Professor and Head of Analytical Chemistry, University of Vienna, Austria



**Frederic Lynen**  
Professor, Separation Sciences Group, University of Ghent, Belgium



**Josephine Bunch**  
Co-Director, National Centre of Excellence in Mass Spectrometry Imaging, NPL and Associate Professor, University of Nottingham, UK



**Ian Wilson**  
Professor and Chair of Drug Metabolism and Molecular Toxicology, Imperial College London, UK



**Christopher Wootton**  
Research Fellow, University of Warwick, UK



**Colin Creaser (Track Chair)**  
Professor of Analytical Chemistry, Loughborough University, UK



**Simon Lambert (Track Chair)**  
Managing Director, ARC Sciences Limited, UK

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08.00-08.50	<b>Registration &amp; Refreshments – Lindbergh Suite Foyer</b>	
08.50-09.00	<b>Global Engage Welcome Address – Lindbergh Room 3</b> <b>Track Chair's Opening Remarks:</b> Simon Lambert MSc, Managing Director, ARC Sciences Ltd	
09.00-09.40	<b>Keynote Presentation - Translational molecular imaging mass spectrometry: from instrumentation to clinical research</b> <ul style="list-style-type: none"> <li>The benefits of high throughput mass spectrometry imaging for molecular pathology</li> <li>Clinical applications of imaging MS</li> <li>New developments in high performance imaging MS</li> </ul> Confirmed: <b>Ron Heeren, Limburg Chair, Professor of Molecular Imaging and Director of M4I (the Maastricht MultiModal Molecular Imaging Institute), Maastricht University, The Netherlands</b>	
09.40-10.15	<b>Keynote Presentation - Unlocking protein primary and higher-order structure by use of 21 tesla fourier transform ion cyclotron resonance mass spectrometry</b> <ul style="list-style-type: none"> <li>Mapping contact surfaces in protein complexes by hydrogen/deuterium exchange monitored by ultrahigh-resolution electrospray ionization FT-ICR mass spectrometry.</li> <li>Protein sequence variants and post-translational modifications (methylation, acetylation, glycosylation, phosphorylation) resolved and identified by top-down HPLC MS/MS: histones, transfer RNA synthetases, cadherin, monoclonal antibodies.</li> <li>Metabolomics: Combination of ultrahigh resolution FT-ICR MS and two-dimensional <sup>1</sup>H/<sup>13</sup>C NMR HSQC and HSQC-TOCSY.</li> </ul> Confirmed: <b>Alan Marshall, Professor of Chemistry and Biochemistry, Florida State University and Chief Scientist, Ion Cyclotron Resonance Program, National High Magnetic Field Laboratory, USA</b>	
10.15-10.45	<b>Solution Provider Presentation - Electrochemical reduction of proteins for enhanced MS and MS/MS capabilities</b> <ul style="list-style-type: none"> <li>Using the ROXY-EC system to achieve effective online electrochemical-reduction of protein disulphide bonds</li> <li>Monitoring the electrochemical reduction process via high-resolution isotope measurements to gain insights into the mechanism of EC reduction</li> <li>Using ROXY-EC reduction to access disulphide bond-protected regions in protein structure and enhance MS/MS analysis</li> </ul> Confirmed: <b>Christopher Wootton, Research Fellow, University of Warwick, UK</b>	
10.45-11.35	<b>Morning Refreshments – Lindbergh Suite Foyer</b> <b>Poster Presentation Sessions</b>	
	<b>Track 1 – Mass Spectrometry: Strategies and Technologies</b> Lindbergh Room 3	<b>Track 2 – Healthcare Case Studies and Applications</b> Lindbergh Room 2
11.35-12.00	<b>Development of a novel acoustic loading system for mass spectrometry applications</b> The high throughput direct measurement of substrate-to-product conversion by label-free detection could be considered the “Holy Grail” of drug discovery screening. Mass spectrometry has the potential to be part of the ultimate screening solution, however, throughput limits it impact. To address this issue we have built a revolutionary acoustic sample delivery system capable of generating an ion beam at rates fast enough to generate ~10,000 data points per hour. The presentation will include details of the development of the prototype system and data from our first 250,000 compound screens. In addition to sharing current biological screening data we will outline potential future applications for this platform including monitoring chemical reactions in real time and high throughput QC of large chemistry libraries. Confirmed: <b>Jonathan Wingfield, Principal Scientist, AstraZeneca, UK</b>	<b>From novel disease mechanisms to predictive biomarkers: combining proteomics and lipidomics for the investigation of metastatic melanoma</b> <ul style="list-style-type: none"> <li>Analysis of proteins and lipids in melanoma tissue and blood samples, primary melanoma cells and cancer-associated fibroblasts by high-resolution mass spectrometry</li> <li>Blood platelets were found to drive late-stage melanoma by the release of lipid survival factors which are detectable in blood plasma</li> <li>A serum protein signature may predict the establishment of resistance against BRAF inhibitors in patients and supports the establishment of novel treatment options</li> </ul> Confirmed: <b>Christopher Gerner, Professor and Head of Analytical Chemistry and Deputy Head of the Mass Spectrometry Centre, University of Vienna, Austria</b>
12.00-12.25	<b>High-throughput analysis of serum (glyco)proteins by various mass spectrometry-based proteomics strategies</b> <ul style="list-style-type: none"> <li>Development of automated and high-throughput mass spectrometry-based methods for exploratory analysis of clinical samples</li> <li>Various mass spectrometry-based proteomics strategies</li> <li>Benefits of ultrahigh resolution mass spectrometry for proteomics</li> </ul> Confirmed: <b>Simone Nicolardi, Senior Researcher, Leiden University Medical Center, The Netherlands</b>	<b>Proteomic analysis of T cell epitopes: Harnessing the immune system to treat cancer</b> Proteomics is a powerful tool for characterizing T cell epitopes that can be used either as diagnostic biomarkers, therapeutic reagents, or as targets for biotherapeutic drug design. Using high throughput mass spectrometric techniques in combination with next generation sequencing and bioinformatic strategies the immune-repertoire can be characterized and novel mutated and immunogenic peptides discovered. This talk will show our current strategies for working with low level materials for the characterization of MHC class I and class II epitopes as well as how we utilize these methods to unravel cellular modulation of the T cell response and how this pertains to the development of cancer vaccines and other initiatives. Confirmed: <b>Jennie Lill, Director, Proteomics and Biological Resources, Genentech, USA</b>
12.25-12.50	<b>Quantitative phosphoproteomics and N-terminomics from clinical samples</b> The analysis of post-translational modifications in clinical samples is often hampered by the limited amount of available sample material. Therefore, we developed robust and sensitive workflows that enable the quantitative analysis of protein phosphorylation and cleavage (N-terminomics) from amounts down to 20 µg per sample. These protocols are applied to study clinical samples such as platelets, CLL cells, or cancer tissues, both in discovery and targeted approaches. Thus, it is possible to quantify 1000s of phosphorylation and cleavage events across multiple clinical samples. Confirmed: <b>Rene Zahedi, Group Leader of Protein Dynamics, ISAS, Germany</b>	<b>Clinical applications of breast cancer proteomics</b> <ul style="list-style-type: none"> <li>Rapid classification of molecular subtypes of breast cancer</li> <li>Development of assays to aid choice of treatment</li> <li>Profiling local and distant recurrences and the consequences for treatment</li> </ul> Confirmed: <b>Peter James, Professor of Protein Technology, Lund University, Sweden</b>

<p><b>12.50-13.20</b></p>	<p><b>Liquid extraction surface analysis mass spectrometry and differential ion mobility mass spectrometry: Tools for scratching the surface</b></p> <ul style="list-style-type: none"> <li>Liquid extraction surface analysis (LESA) mass spectrometry is suitable for the analysis of intact proteins from a range of biological substrates and can be applied for mass spectrometry imaging.</li> <li>Native LESA mass spectrometry enables the analysis of protein complexes.</li> <li>LESA may be coupled with differential ion mobility mass spectrometry (also known as FAIMS) for improved protein analysis, and FAIMS is a suitable tool for inclusion in mass spectrometry imaging workflows.</li> </ul> <p>Confirmed: <b>Helen Cooper, Professor of Mass Spectrometry, University of Birmingham, UK</b></p>	<p><b>In depth mass spectrometric characterization of locked-nucleotidic acids (LNA) - a new class of versatile drugs</b></p> <p>The presentation will introduce a new class of pharmaceutical drugs and will show the wide range of potential applications. Analytical challenges of synthetic oligonucleotides above a mass of 5000 Da will be shown and how high resolution mass spectrometry can help developing new drug molecules and may lead to new synthetic routes.</p> <p>Confirmed: <b>Joerg Hoernschemeyer, Head of Mass Spectrometry Laboratory for Peptides, Oligonucleotides and Proteins, Preclinical CMC, Roche Innovation Centre, Basel, Switzerland</b></p>
<p align="center"><b>Lunch – Lindbergh Suite Foyer</b></p>		
<p align="center">Track Chair: Colin Creaser, Professor of Analytical Chemistry, Loughborough University, UK</p>		
<p><b>14.20-14.45</b></p>	<p><b>Dynamic protein structure: from protein disorder to membrane pores</b></p> <p>This lecture focuses on aspects of dynamic and heterogeneous protein conformations and assemblies, using an integrated structural approach based on "native" mass spectrometry, ion mobility, and other biophysical methods. Specifically, we show recent results on the detection and characterization of intrinsic disorder in proteins, including alpha-synuclein. These data link the conformational state of the protein with their association into larger oligomers and fibrils. We also use detergent micelles and nanodiscs for native MS studies of different ion channels including the mechanosensitive channel of large conductance (MscL). Using covalently attached, charged ligands inside the pore, we can mimic the effect of mechanical pressure on the surrounding membrane and characterize various opening states using ion mobility-MS, electron microscopy, EPR spectroscopy and other biochemical and computational methods.</p> <p>Confirmed: <b>Frank Sobott, Professor of Biomolecular and Analytical Mass Spectrometry, University of Antwerp, Belgium</b></p>	<p><b>Integrated glycoproteomics pipeline for discovery and validation of differentially glycosylated serum proteins as cancer biomarkers</b></p> <p>Translation of biomarkers discovered from proteomics studies have been challenging, possibly due to variability of sample processing and the complexity of body fluid proteomes. To facilitate cancer diagnosis and management through new biomarkers for blood tests, we developed an integrated pipeline for efficient serum glycoprotein biomarker discovery and verification, without the need to deplete abundant serum proteins. The pipeline uses semi-automated lectin magnetic bead array (LeMBA)-coupled tandem mass spectrometry with a dedicated data-housing and analysis pipeline for biomarker selection (GlycoSelector). This presentation will report its application in the discovery and validation of oesophageal cancer biomarkers in independent cohorts. While the candidate biomarkers require further large-scale clinical evaluation, an important feature of the pipeline is the potential for rapid translation of the candidate biomarkers to lectin-immunoassays.</p> <p>Confirmed: <b>Michelle Hill, Associate Professor and Head of the Cancer Proteomics Group, University of Queensland Diamantina Institute, Australia</b></p>
<p><b>14.45-15.10</b></p>	<p><b>Quan-Qual analysis using high-resolution mass spectrometry: a paradigm shift or just common sense?</b></p> <p>New generation high-resolution MS (HRMS) systems offer the right performance, i.e., sensitivity, dynamic range, resolution, accuracy and scan-to-scan reproducibility, for quantitative analyses. The most recently released HRMS systems show further advancements in user friendliness, foot print and price making these a worthwhile alternative for triple quadrupole MS systems. HRMS analyses can be easier to setup (no fragmentation) but, most importantly, provide the potential to combine quantitative and qualitative analyses (quan-qual). This results in a huge potential but also requires more experience and data mining to make the right choices to come to the best results. The advantages, challenges and tips and tricks for high-resolution MS based quantification and quan/qual analysis will be discussed.</p> <p>Confirmed: <b>Filip Cuyckens, Scientific Director &amp; Fellow, Pharmacokinetics, Dynamics &amp; Metabolism, Janssen R&amp;D, Belgium</b></p>	<p><b>Combining mass spectrometry approaches for elucidating the structure and function of proteins containing large unstructured regions</b></p> <p>Over 30% of all eukaryotic proteins are either completely disordered or contain large parts of intrinsically disordered regions. They can obtain multiple conformations and play important roles within the cell, however, their study poses problems for traditional structural biology methods. We show that a combination of structural mass spectrometry techniques can be used to successfully study the structure of such proteins. Underpinning these measurements are computational methods that can make use of and effectively integrate such data. We present a new computational approach for handling chemical crosslinking data and use our experimental and computational methodologies to study the protein human histone deacetylase 2 (HDAC2), a protein involved in regulation of gene expression which is vital in development, some cancers and neurodegenerative disorders.</p> <p>Confirmed: <b>Konstantinos Thalassinos, Senior Lecturer in Biophysical Mass Spectrometry, University College London, UK</b></p>

15.10-15.35	<p><b>Imaging of complex systems, across the mass and length scales</b></p> <ul style="list-style-type: none"> <li>• MALDI, SIMS and ambient MS imaging methods for biomedical research</li> <li>• Developing metrology for 2D and 3D imaging of small and large molecules</li> <li>• Towards a 'google-earth' view of tissue biochemistry</li> </ul> <p>Confirmed:  <b>Josephine Bunch, Co-Director of the National Centre of Excellence in Mass Spectrometry Imaging, and Associate Professor, University of Nottingham, UK</b></p>	<p><b>Chemical crosslinking to investigate intracellular protein interactions in the nucleus</b></p> <p>Structural investigations into protein-to-protein interactions can be readily achieved by combining chemical crosslinking of proteins with mass spectrometric analyses. With this technique detailed information can be obtained on the interaction interfaces and to date mostly highly purified protein complexes have been investigated. Recent advances in mass spectrometry performance have however dramatically expanded the scope to more complex mixtures. This lecture will focus on data analysis software implemented in Proteome Discoverer and its application to the elucidation of the protein-protein interaction networks in the nucleus.</p> <p>Confirmed:  <b>Richard Scheltema, Junior Assistant Professor, University of Utrecht, The Netherlands</b></p>
15.35-16.00	<p><b>Integrative deep proteo-metabolome profiling of cancer cell energy homeostasis</b></p> <p>Metabolic reprogramming of solid tumours responds to a severe microenvironment that is characterized by low oxygen tension and an inadequate supply of nutrients. To address underlying molecular changes at a systems level, we utilised spheroid culture and HIF-1a knockout cell models to better mimic the solid tumour microenvironment. We collected and integrated transcriptome, deep-proteome, metabolome and fluxome analyses to profile the hypoxic energetic metabolism of hypoxic colorectal cancer cells grown in 2D and 3D cultures. Our results indicate a switch from ATP to phosphocreatine (PCr)-dependent energy pathways to maximise multidimensional growth.</p> <p>Confirmed:  <b>Benedikt Kessler, Professor of Biochemistry and Life Science Mass Spectrometry, University of Oxford, UK</b></p>	
16.00-16.50	<p align="center"><b>Afternoon Refreshments – Lindbergh Suite Foyer Poster Presentation Sessions</b></p>	
16.50-17.15	<p><b>Mass spectrometry imaging in drug delivery studies</b></p> <p>Mass spectrometry imaging (MSI) enables highly specific imaging of exogenous as well as endogenous compounds in tissue samples. The presentation will provide examples of the use of DESI-MSI and MALDI-MSI for distribution studies of drug and drug metabolites over different tissue barriers, including skin, as well as in whole-body studies.</p> <p>Confirmed:  <b>Christian Janfelt, Associate Professor and PI of the Mass Spectrometry Imaging Laboratory, University of Copenhagen, Denmark</b></p>	
17.15-17.40	<p><b>Antibody-independent, highly sensitive targeted proteomics methods for preclinical verification of biomarkers</b></p> <ul style="list-style-type: none"> <li>• Targeted mass spectrometry for preclinical biomarker verification</li> <li>• Development of antibody-independent, highly sensitive targeted proteomics methods</li> <li>• Applications of the advanced targeted proteomics platforms</li> </ul> <p>Confirmed:  <b>Tao Liu, Senior Staff Scientist, Pacific Northwest National Laboratory, USA</b></p>	
17.40	<p align="center"><b>Chair's Closing Remarks and End of Day 1</b></p>	
17.45-18.45	<p align="center"><b>Networking Drinks Reception – Lindbergh Suite Foyer</b></p> <p align="center">If you would like to sponsor the drink's reception please contact Faizel Ismail at <a href="mailto:faizel@globalengage.co.uk">faizel@globalengage.co.uk</a></p>	

08.20-08.55	Refreshments – Lindbergh Suite Foyer	
08.55-09.00	Global Engage Welcome Address – Lindbergh Room 3 Track Chair's Opening Remarks: Simon Hubbard, Professor of Computational Biology, University of Manchester, UK	
09.00-09.40	Keynote Presentation <b>Mass spectrometry of membrane proteins – the lipid connection</b> <ul style="list-style-type: none"> <li>• Study of membrane proteins by mass spectrometry</li> <li>• New information in relation to lipid and drug binding</li> <li>• New vehicles for delivery into the gas phase and prospects for novel instrumentation</li> </ul> Confirmed: <b>Dame Carol Robinson, Dr. Lee's Professor of Chemistry, University of Oxford, UK</b>	
	<b>Track 1 – Mass Spectrometry Related Methodologies</b> Track Chair – Simon Hubbard, University of Manchester Lindbergh Room 3	<b>Track 2 – Healthcare Case Studies and Applications</b>  Lindbergh Room 2
09.40-10.05	<b>An overview of the PRIDE ecosystem of resources and computational tools for mass spectrometry proteomics data</b> <ul style="list-style-type: none"> <li>• Overview of the PRIDE Archive as the world-leading proteomics data repository, and its related stand-alone tools (especially PRIDE Inspector).</li> <li>• Introduction of the ProteomeXchange Consortium, aiming to standardise data submission and dissemination worldwide.</li> <li>• Current examples of public proteomics data reuse, including some of our own work in this topic (the PRIDE Cluster resource).</li> </ul> Confirmed: <b>Juan Antonio Vizcaino, Proteomics Team Leader, European Bioinformatics Institute, European Molecular Biology Laboratory, UK</b>	<b>Development of a mass spectrometry platform to enhance clinical research</b> Proteomic profiling of tissues and biofluids with relatively high throughput offers great opportunities to define biomarkers of risk, prognosis, toxicity and diagnosis plus disease mechanism. The use of techniques like SWATH mass spectrometry (MS) and Selected Reaction Monitoring MS therefore have a great deal to offer precision medicine approaches. We have a clinical proteomics centre with 13 mass spectrometers to realise this potential. The system is fully integrated with health informatics to ensure the swiftest possible generation of new clinically relevant information for earlier patient benefit.  Confirmed: <b>Tony Whetton, Director, Stoller Biomarker Discovery Centre and Director, Manchester Precision Medicine Institute, UK</b>
10.05-10.30	<b>Identification of pathogenic microorganisms using MALDI-TOF mass spectrometry and in silico spectral databases</b> The last ten years have seen the advent of MALDI-TOF MS as a new tool for microbial identification in the clinical routine. MALDI TOF MS identification of microorganisms depends strongly on the quality of mass spectral libraries which have to be acquired under standardized conditions (cultivation, sample preparation, data acquisition). In the context of the ever-increasing amount of bacterial whole genome data, we have initiated a project to compile an in silico database from protein sequences data contained in the publicly available SwissProt and TrEMBL databases. The in silico database is manufacturer independent and currently contains entries derived from approx. 10.800 microbial genomes. Preliminary tests of the database suggest that the bioinformatics-based strategy allows microbial identification at the genus and at the species level.  Confirmed: <b>Peter Lasch, Group Leader, Robert Koch Institute, Germany</b>	<b>Measuring (human) tumor specific protein synthesis using MS and MSI techniques</b> Using a primed continuous infusion of stable isotopically labelled phenylalanine we were able to measure fractional synthetic rates (FSR) of protein synthesis rates (of pancreatic cancer, pancreatic tissue, intestinal, hepatic and (2 types of) muscle tissue in patients undergoing surgery. Using the same tracers, we were also able to measure tracer/tracee ratios of phenylalanine at the tumour level using Imaging MS, enabling us to 'visualize' tumour clone specific FSR.  Confirmed: <b>Steven Olde-Damink, Professor of Surgery and Director of Research Laboratories, Maastricht University, The Netherlands</b>
10.30-11.20	Morning Refreshments – Lindbergh Suite Foyer Poster Presentation Sessions	
11.20-11.45	<b>The bottom to top of signaling using mass spectrometry</b> Intracellular protein signalling is extensively mediated by protein post-translational modifications (PTMs). Peptide-based mass spectrometric (MS) analysis, or 'bottom-up' proteomics, has been used successfully for a number of years to identify these sites of modification. However, these types of qualitative analyses do not typically permit understanding of how different PTMs are dynamically regulated and also how different sites of modification on a single protein may be co-regulated. We demonstrate the utility of combining peptide 'bottom-up' and protein-based 'top-down' (ion mobility-)MS analyses of NF-κB to help elucidate novel regulatory mechanisms of the NF-κB signalling system, a critical pathway mediating (amongst other things) cellular responses to inflammation and DNA damage.  Confirmed: <b>Claire Eyers, Professor of Biomolecular Mass Spectrometry and Co-Director of the Centre for Proteome Research, University of Liverpool, UK</b>	<b>Mass spectrometry imaging standardisation in the Mannheim Molecular Intervention Environment (M<sup>2</sup>OLIE)</b> The "Mannheim Molecular Intervention Environment (M <sup>2</sup> OLIE)" is one of nine public-private partnerships for Innovation initiated by the German Ministry of Education and Research. In interdisciplinary fashion, M <sup>2</sup> OLIE develops an integrated, innovative medical intervention environment for the development of minimally invasive cancer treatments. As part of this development, therapeutic procedures are being improved and assisted by multimodal <i>in-vivo</i> imaging methods, robot-based intervention assistants, mass spectrometry imaging-based tumor classification, and patient-specific radio-theranostics. Eventual clinical use of very complex mass spectrometry imaging workflows requires rigorous standardization of methods. Therefore, in addition to introducing the M <sup>2</sup> OLIE intervention environment, this talk will present experimental set-ups and new statistical scores for standardization of future clinical mass spectrometry imaging of biopsies.  Confirmed: <b>Carsten Hopf, Professor and Head of the Research Center for Applied Biomedical Mass Spectrometry (ABIMAS), Mannheim University of Applied Sciences, Germany</b>

<p>11.45-12.10</p>	<p><b>Top-down proteomics of bacterial pathogens</b>                  In the last decade, the development of MALDI-TOF MS for rapid microbial identification has revolutionized the field of clinical microbiology. By simply comparing a spectral protein profile obtained from the analysis of a bacterial colony to a large database of reference spectra, species identification can be achieved. However, some bacterial pathogens remain difficult to identify, either because they do not give a specific profile or because the database lacks the appropriate reference. In addition, the discriminatory power of MALDI-TOF is often insufficient for differentiating sub-species within species or clones within sub-species. We show here that top-down proteomics provides a nice alternative allowing an efficient and accurate microbial characterization even for bacterial pathogens giving undistinguishable MALDI-TOF signatures. Top-down proteomics is an emerging technology based on the analysis of intact proteins using high-resolution mass spectrometry.</p> <p>Confirmed:  <b>Julia Chamot-Rooke, Head of Structural Mass Spectrometry, Institut Pasteur, France</b></p>	<p><b>Unravelling the mechanistic basis of intrinsic drug resistance in mycobacteria through proteomics</b>                  Mycobacterium tuberculosis - the causative agent of tuberculosis disease - kills ~1.5 million people annually and drug resistant strains are spreading. Poor penetration of granulomas by specific antibiotics mean M. tuberculosis bacilli may face sub-lethal drug doses at the site of disease.                  We have quantified time-dependent changes in the proteome of the non-pathogenic model organism, M. smegmatis, in the presence of sub-lethal concentrations of rifampicin, analysing time-points corresponding to early response, onset of bacteriostasis and early recovery. After dampening an initial SOS response, we found that the bacteria suppress the DosR regulon, upregulate both transcriptional and translational machinery, and dysregulate haeme and mycobactin synthesis. Later, upregulation of the M. smegmatis specific rifampin ADP-ribosyl transferase creates phenotypic drug resistance as a likely prelude to genotypic resistance.</p> <p>Confirmed:  <b>Jonathan Blackburn, Research Chair, Applied Proteomics and Chemical Biology, University of Cape Town, South Africa</b></p>
<p>12.10-12.35</p>	<p><b>Novel strategies for the elimination of matrix effects in pharmaceutical LC-MS</b>                  Analysis of drugs and metabolites in biological matrices such as blood or plasma by LC-MS is routinely challenged by the presence of large quantities of competing molecules for ionization in soft ionization sources, such as proteins and phospholipids. While the former can easily be removed by protein precipitation, pre-analytical extraction of the latter is necessary because they show very high retention in reversed-phase LC resulting in long analysis times or in ion suppression effects when not eluted before the next runs. Complementary HILIC based SPE approaches making use of silica cartridges and of acetone as organic solvent, are proposed in this work as potent alternatives to current commercial methods for phospholipid removal. The methodologies were developed and tested for a broad polarity range of pharmaceutical solutes (log P from 0 to 6.6) allowing broader implementation in biomedical analysis.</p> <p>Confirmed:  <b>Frederic Lynen, Professor of Separation Sciences, University of Ghent, Belgium</b></p>	<p><b>MS-based adenovirus proteomics</b>                  Human adenovirus is a widely model system for studying infection. The extent of posttranslational modifications (PTMs) on the viral proteins and their biological significance remain to be determined. PTMs are added to proteins after their translation and have impact on their structure, function and their involvement in signal transduction. We were the first group reporting PTMs in an intact viral particle. In current projects we present analytical strategies to reveal phosphorylations of Ad2 non-structural proteins. Furthermore, we investigate the host cellular gene expression in the response to viral infection at the protein and PTM levels. Our results show that the regulation is more complex than hitherto believed and several examples of posttranscriptional regulation of gene expression were observed.</p> <p>Confirmed:  <b>Sara Lind, Associate Professor, Uppsala University, Sweden</b></p>
<p>12.35-13.00</p>	<p><b>Liquid chromatography combined with ion mobility and mass spectrometry for metabolic phenotyping</b>                  Liquid chromatography (LC), combined with mass spectrometry (MS) is widely now used for both targeted and untargeted metabolic phenotyping. As with all of the analytical methods used for this type of work, the desire for comprehensive metabolic profiles of metabolites has to be balanced against the need to generate them rapidly, reproducibly and efficiently. One means of increasing the “analytical space” available for the detection of metabolites, without increasing the analysis time, is to combine LC with ion mobility spectrometry (IMS) to provide an extra dimension of separation prior to mass spectrometry. The potential of LC-IMS-MS for metabolic phenotyping tool will be discussed and illustrated with examples.</p> <p>Confirmed:  <b>Ian Wilson, Professor and Chair of Drug Metabolism and Molecular Toxicology, Imperial College London, UK</b></p>	<p><b>Medical diagnosis / prognosis based on Fe and Cu isotope ratios in human biofluids</b></p> <ul style="list-style-type: none"> <li>• Use of high-precision isotopic analysis of essential transition metals in human biofluids using multi-collector ICP-mass spectrometry</li> <li>• The isotopic composition of serum Fe reflects the iron status in sickness and health</li> <li>• The isotopic composition of serum Cu is measurably and systematically affected in the case of liver disease and shows promise as a diagnostic/prognostic biomarker</li> </ul> <p>Confirmed:  <b>Frank Vanhaecke, Professor of Analytical Chemistry, Ghent University, Belgium</b></p>
<p>13.00-14.00</p>	<p>Lunch – Lindbergh Suite Foyer</p>	
<p>14.00-14.25</p>	<p><b>Quantitative proteomics workflows to monitor the impact of specific protein kinase inhibitors on regulatory kinase networks and the phosphoproteome.</b></p> <ul style="list-style-type: none"> <li>• Emergence of protein kinase inhibitors for therapeutic applications</li> <li>• Quantitative proteomic workflows can monitor the impact of kinase inhibitors on the kinome and phosphoproteome</li> <li>• Specific kinase inhibitors elicit dramatic changes within the kinome and phosphoproteome reflecting a high level of integration within regulatory kinase networks</li> </ul> <p>Confirmed:  <b>David Litchfield, Professor and Chair of Biochemistry, University of Western Ontario, Canada</b></p>	



14.25-14.50	<p><b>Proteomics at clinical scale for biomarker discovery in human plasma and cerebrospinal fluid</b>                  Mass spectrometry-based proteomics can characterize human plasma and cerebrospinal fluid (CSF) proteomes to a great extent. Deep proteome coverage comes nonetheless with important limitations in terms of analysis time which is a critical factor for clinical studies. As the analysis of a sufficient number of samples is compulsory to empower statistically-robust candidate biomarker findings, we have developed a scalable automated proteomic pipeline, so-called ASAP<sup>2</sup>, to enable the proteomic analysis of large numbers of plasma and CSF samples (i.e., &gt; 100-1000).                  This human body fluid profiling approach was applied to metabolic and brain health research projects. Potential biomarkers were identified in those studies for clinical purposes, but also more general proteome observations could be made and replicated at the population level.</p> <p>Confirmed:  <b>Loïc Dayon, Proteomics Team Leader, Nestlé Institute of Health Sciences, Switzerland</b></p>
14.50-15.15	<p><b>The use of metabolomics in the study of embryo growth and neonatology</b>                  IVF success rates remain relatively low. The metabolic content of embryo culture media could provide useful information related to its viability. Pre-term birth remains a major health problem. Mapping different biological fluids, obtained from pregnant women, could allow useful correlations with the fate of the pregnancy. Preterm neonates spend weeks in Intensive care units where nosocomial infections may cause morbidity including necrotising enterocolitis and sepsis.                  More than 3000 samples (IVF culture medium, maternal blood/urine, amniotic/coelomic fluid from women, blood and urine from neonates) were analysed in Holistic and targeted metabolomics. Here we present results that correlate metabolome with health state and show that metabolomics provide potential for the assessment of embryo viability before implantation, its growth during pregnancy and in neonatology.</p> <p>Confirmed:  <b>Georgios Theodoridis, Professor of Chemistry, Aristotle University, Thessaloniki, Greece</b></p>
15.15-15.45	<p style="text-align: center;"><b>Afternoon Refreshments – Lindbergh Suite Foyer                  Poster Presentation Sessions</b></p>

## Venue

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### Poster Presentations – A few examples are below

Title	Principal Author(s)	Affiliation
1 UPLC Method for Determination of Eight Flupirtine Impurities in Bulk Samples and their Characterization by <sup>1</sup> H NMR & ESI-MS	Dr. Ms. Anna Pratima Nikalje, Mr. Dileep Bhosale	Y.B. Chavan College of Pharmacy, Aurangabad.MS.India
2 How to spot cocaine consumption in the greater Tunis area by analyzing its major metabolite benzoylecgonine in wastewater? Utility in Forensic Epidemiology	Bilel Moslah (Ph.D student)	Faculty of Pharmacy of Monastir
3 MALDI MS Imaging with Scanning Laser Beam	Antonín Bednařík <sup>1,2</sup> , Markéta Machálková <sup>2</sup> , Kateřina Coufalíková <sup>2</sup> , Pavel Houška <sup>3</sup> , Eugene Moskovets <sup>4</sup> , Jarmila Navrátilová <sup>5</sup> , Jan Šmarda <sup>5</sup> , Jan Preisler <sup>1,2</sup>	<sup>1</sup> Department of Chemistry, Masaryk University, Brno, Czech Republic <sup>2</sup> CEITEC, Masaryk University, Brno, Czech Republic <sup>3</sup> FME, University of Technology, Brno, Czech Republic <sup>4</sup> MassTech, Inc., Columbia, MD <sup>5</sup> Department of Experimental Biology, Masaryk University, Brno, Czech Republic
4 Scout-MRM : extended portability of large multiplexed peptide assay	Blandine Rougemont, Romain Carriere, Sophie Aycirix, Dave Cox, Sebastien Bontemps Gallo, Jean-Marie Lacroix, Yves LeBlanc, Jerome Lemoine	Universite Lyon1, France
5 Structural and functional insights in ciprofloxacin- versus imipenem-induced membrane vesicle secretion by the multidrug resistant species <i>Stenotrophomonas maltophilia</i>	Wouter Van Putte, Jolien Vitse, Gonzalez Van Driessche, Stephan Stremersch, Wim Van Den Broek, Koen Raemdonck, Kevin Braeckmans, Henning Stahlberg, Misha Kudryashev, Savvas Savvides, Bart Devreese	Ghent University
6 SMALP Lipidomics: An Investigation Into the Lipid Profile of Key Bacterial Cell Division Membrane Proteins	Alvin C. K. Teo <sup>1</sup> , Sarah C. Lee <sup>2</sup> , Naomi L. Pollock <sup>2</sup> , Alpesh Thakker <sup>3</sup> , Rosemary A. Parslow <sup>2</sup> , Stephen C. Hall <sup>2</sup> , Andrew R. Pitt <sup>3</sup> , Timothy R. Dafforn <sup>2</sup> , , Corinne M. Spickett <sup>3</sup> , David I. Roper <sup>1</sup>	<sup>1</sup> School of Life Sciences, Gibbet Hill Road, University of Warwick, Coventry, CV4 7AL, UK <sup>2</sup> School of Biosciences, University of Birmingham, Edgbaston, Birmingham, B15 2TT, UK <sup>3</sup> School of Life and Health Sciences, Aston University, Aston Triangle, Birmingham, B4 7ET, UK

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