Scottish Metabolomics Network Meeting 2016

Centre for Health Science, Inverness

16th and 17th November 2016

Delegate Programme Booklet

Welcome and Introduction

We extend a very warm welcome to all delegates to the University of the Highlands and Islands in Inverness for the Scottish Metabolomics Network Meeting 2016. The network was established with the aim of encouraging the exchange of experiences and ideas between researchers based at Scottish Universities who are working in the field of metabolomics (and in some cases lipidomics).

The two day meeting will discuss advances and challenges in metabolomic analysis and its applications. There are a range of presentations and posters from seasoned academics as well as early stage career researchers and PhD students based at institutions throughout Scotland. Colleagues from industry will also be highlighting some of their latest developments.

We would like to take this opportunity to thank all of our sponsors whose support has been crucial in allowing us to organise the meeting as well as The Highland Council, which is hosting a Civic Dinner for delegates. We very much hope that you will find the meeting enjoyable and that there are opportunities to make new contacts and build collaborative links.

Phillip Whitfield and Mary Doherty
University of the Highlands and Islands

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Day One - PROGRAMME

10.30 – 11.10	Registration, Refreshments
11.10 – 11.15	Welcome by Phil Whitfield
11.15 – 11.25	Introduction to Scottish Metabolomics Network - Karl Burgess
11.25 – 13.00	***Scientific Session 1 - Pipelines and Workflows*** **CHAIR: Mary Doherty**
11.25 – 11.45	**Dave Watson (University of Strathclyde)** ***Derivatisation strategies for enhanced and detection and separation in metabolomics studies***
11.50 – 12.10	**Karl Burgess (University of Glasgow)** ***Metabolomics in space and time***
12.15 – 12.35	**Gillian Mackay (Beatson Institute for Cancer Research)** ***An untargeted approach to metabolomics with Progenesis QI software***
12.40 – 13.00	**Thermo Fisher Scientific** **Anas Kamleh** ***Orbitrap Tribrid: A Trinity of Mass Analyzers for Successful Metabolomics Discovery***
13.00 – 14.00	Lunch, Poster Viewing and Networking
14.00 – 15.35	***Scientific Session 2 - Metabolomics in Biology I*** **CHAIRS: Ruth Andrew and Natalie Homer**
14.00 – 14.20	**Wendy Russell (Rowett Institute of Nutrition and Health, University of Aberdeen)** ***Diet and the human gut metabolome***
14.25 – 14.45	**Oliver Maddocks (University of Glasgow)** ***Cancer specific amino acid metabolism***
14.50 – 15.10	**Simon Young (University of St Andrews)** ***Characterising the essential trypanosomatid lysosome using various mass spectrometric techniques***
15.15 – 15.35	**Waters** **Lidia Jackson** ***Utilizing an IMS-DIA-MS Workflow to Characterize and Quantify the Obesity and Diabetes Lipidome***
15.35 – 16.05	Coffee, Poster Viewing and Networking

Day One - PROGRAMME

16.05 – 17.30 ***Scientific Session 3 - Software and Bioinformatics***
CHAIR: Phillip Whitfield

16.05 – 16.25 **Simon Rogers (University of Glasgow)**
MS2LDA: Decomposing mass spectra with tools from text mining

16.30 – 16.50 **Jimi Wills (University of Edinburgh)**
Simple tools in assays, identification and quantification

16.55 – 17.15 **Agilent Technologies**
Anthony Sullivan
Combining Flux Analysis with Cellular Bioenergetics – Agilent's Powerful New Combinations

17.15 – 17.30 Discussion and Close

Civic Dinner Hosted by The Highland Council

Start Time: 19:00-19:30

Venue: The Kingsmills Hotel

Address: Culcabock Road, Inverness IV2 3LP

Day Two - PROGRAMME

09.20 – 10.30 ***Scientific Session 4 - Targeted Metabolite Analysis***
CHAIR: Andy Finch

09.20 – 09.40 **Kerstin Ziegler (University of the Highlands and Islands)**
Method validation for targeted analysis of endogenous lipid mediators

09.45 – 10.05 **Shazia Khan (University of Edinburgh)**
Derivatisation of steroids to enhance sensitivity and isomer separation

10.10 – 10.30 **Sciex**
Stephen Ayris
The Lipidyzer™ Platform: A Revolutionary Tool for Understanding the Role of Lipids in Disease

10.30 – 11.00 Coffee, Poster Viewing and Networking

11.00 – 12.35 ***Scientific Session 5 - Metabolomics in Biology II***
CHAIR: Karl Burgess

11.00 – 11.20 **Joy Edwards-Hicks (University of Edinburgh)**
Evasion of tumour suppression by Myc-driven cancer

11.25 – 11.45 **Will Allwood (James Hutton Institute)**
Targeted and non-targeted metabolite profiling in plants and foods, and why targeted is not always for the best

11.50 – 12.10 **Rebecca Goss (University of St Andrews)**
Blending synthetic chemistry and synthetic biology to make new to nature natural products

12.15 – 12.35 **Shimadzu**
Christopher Titman
Exploring Changes in Primary Metabolites in Alzheimer's Disease using Targeted LC-MS/MS

12.35 – 13.30 Lunch, Poster Viewing and Networking

13.30 – 14.30 **Keynote Address**
Professor Matthew Dalby (University of Glasgow)
Metabolomics in mesenchymal stem cell biomaterials and cell engineering research

14.30 – 15.00 Closing Remarks, Poster Prizes and Announcement of 2017 Meeting

Speaker Biographies

Dr Will Allwood

Research Scientist, James Hutton Institute

During his PhD and ensuing post-doctoral positions Will has become an internationally recognised researcher in the field of metabolomics and metabolite profiling. Will is interested in the study and development of chromatography - linked - mass spectrometry (LC and GC) for a range of applications in the fields of natural product discovery, pharmacology and the human clinical sciences, as well as plant-physiology, pathology and insect interactions. Specific research he has performed includes studies on several molecular plant pathology systems where the aim was to uncover the metabolic basis behind pathogen invasiveness and host immunity. Following his PhD, Will largely developed and applied chromatography - mass spectrometry metabolomics technologies (both non-targeted profiling and quantification of specific target compounds) to the study of nutritional and flavour qualities in fruits and cereals as part of the EU Framework VI META-PHOR project (http://www.meta-phor.eu/). Will has run and provided metabolic profiling services within the Universities of Manchester and Birmingham across many human clinical studies, with particular focus on the discovery of prognostic biomarkers of cancer (principally lung and breast cancers), but also sepsis, hypertension, and cardiomyopathy, to name but a few diseases and conditions. As well as disease biomarker discovery, other applications have included the study of the metabolism of antibiotics in susceptible and resistant bacterial isolates, and studying the actions of commercial and newly developed pharmaceuticals in mammalian cell lines and animal models for specific diseases. Will has also developed key skills in experimental design and quality assurance, sample generation, extraction, chromatography-MS analysis (LC-MS and GC-MS), data processing, metabolite annotation and identification, statistical analysis, network analysis and interpretation of results.

Dr Karl Burgess

Senior Research Fellow, University of Glasgow

Dr Karl Burgess (Glasgow Project Lead) is an internationally recognised expert in metabolomics. A senior research fellow at the University of Glasgow, Dr Burgess established the Glasgow Polyomics Metabolomics Facility 8 years ago and during that time he has published over 40 papers in the field. He is the Chair of the Scottish Metabolomics Network – a grouping of the key biological small molecule researchers in Scotland, and he is also a Key Opinion Leader for ThermoFisher Scientific.

Professor Mathew Dalby
Chair of Cell Engineering, University of Glasgow

Matt Dalby is Professor of Cell Engineering at the University of Glasgow. After a PhD in biomedical materials at Queen Mary, University of London, he moved to Glasgow as a PDRA on EU grant Nanomed where he investigated cell responses to nanoscale features. In 2003 he was awarded a BBSRC David Phillips Fellowship to study mesenchymal stem cell response to nanotopography and to understand cellular mechanotransduction leading to papers in Nature Materials in 2007 and 2011. He has won several early career awards including from NEXXUS, Society for Experimental Biology and the Tissue and Cell Engineering Society. He is currently funded by BBSRC, EPSRC, MRC, Leverhulme Trust and Find a Better Way and has published over 140 papers in the field of cell response to materials. He is more an abuser of metabolomics that a user, with an interest in metabolic differences between growing and differentiating stem cells. However, this abuse of the power of metabolomics has led to some interesting work in bioactive metabolite discovery and understanding how mesenchymal stem cells can be grown better *in vitro* as will be discussed.

Miss Joy Edwards-Hicks
PhD Student, University of Edinburgh

Joy is a final year PhD student at the Institute of Genetics and Molecular Medicine in Edinburgh. The focus of her PhD project has been to understand metabolic stresses induced by oncogene activation. She has interrogated this question through a number of techniques including siRNA screening and LC-MS. Joy's work has involved setup of isotope tracer analysis, as well as method development to identify lipids by subclass.

Dr Rebecca Goss
Reader, University of St Andrews

Dr Rebecca Goss is interested in the biosynthesis of natural products and in how these biosynthetic pathways may be harnessed in order to generate new designer natural products. For analogue generation, this approach can prove more expeditious that total synthesis. Dr Goss completed her undergraduate studies in Chemistry at the University of Durham between 1994-1997. A PhD was then carried out into the biosynthesis of various natural products including the stereochemistry of enzymatic fluorination in fluoroacetate biosynthesis under the supervision of Professor David O'Hagan (University of Durham, awarded 2001). In 2000 Dr Goss moved to the University of Cambridge to study the chemistry and molecular biology of polyketide biosynthesis in the research group of Professors Jim Staunton FRS and Peter Leadlay FRS. In 2002, Dr Goss moved to an independent position within the department of Chemistry at the University of Nottingham. Following the award of a Royal Society BP Dorothy Hodgkin Fellowship in 2003 she moved to the University of Exeter. The Goss research group then moved to the University of East Anglia in 2005. In 2007 Dr Goss was awarded the RSC Meldola prize for "her excellent contributions at the interface of organic chemistry and molecular biology". THE 2013 Natural Product Report Emerging Researcher Lectureship"Awarded for our pioneering new approach to natural product analogue generation "Genochemetics", which marries together Synthetic Biology and Synthetic Chemistry to access new bioactives of medicinal interest", and in 2014 an ERC consolidator award.

Dr Shazia Khan

Postdoctoral Research Associate, University of Edinburgh

Shazia Khan is a postdoctoral researcher in the Centre for Cardiovascular Science, Queen's Medical Research Institute, University of Edinburgh, since 2014, working with Ruth Andrew, Brian Walker and Natalie Homer. After her Ph.D. in Natural Products Chemistry, in 2009, from H. E. J. Research Institute of Chemistry, University of Karachi, Pakistan, she became an Assistant Professor at the COMSATS Institute Pakistan till 2010. During 2011-2014, Shazia has worked as a research assistant at Bioscience Department - Swansea University on fungal secondary metabolites analysis by GC-MS and as a visiting scholar at Strathclyde Institute of Pharmacy and Biomedical Sciences on LC-MS based metabolomics profiling. Shazia has several years' experience of work on natural products purification, structure characterization, synthesis modification and analysis of biologically active analytes by using advanced chromatographic and spectroscopic methods. Most recently she worked on MRC project to develop a diagnostic approach by mass spectrometry imaging to quantify estrogens in tissue samples. Currently she is working on a Wellcome Trust project and developing analytical methods to measure glucocorticoid hormones in tissue samples by high resolution mass spectrometry imaging. She is exploring different derivatising approaches to boost sensitivity of steroids by ESI, MALDI and discriminate isomers by Ion mobility mass spectrometry.

Dr Gillian Mackay

Head of Metabolomics, Beatson Institute for Cancer Research

Gillian has run the metabolomics facility at the Beatson Institute for nearly 5 years, supporting the cancer metabolism research groups, mainly using LC-MS techniques with Exactive and Q-Exactive mass spectrometers, for both targeted and untargeted approaches. Previously Gillian worked at CXR Biosciences, a small Contract Research Organisation, using LC-MS/MS for DMPK studies for preclinical drug development. She obtained her PhD at the University of Glasgow, using HPLC in the field of neuroscience.

Dr Oliver Maddocks

CRUK Research Fellow, University of Glasgow

Oliver started his lab at the University of Glasgow in 2015 funded by Career Development Fellowship from CRUK. His group works on translational cancer metabolism with focus on cancer specific amino acid metabolism. He was previously a post-doctoral researcher at the CRUK Beatson Institute in Glasgow and prior to which he was a post-doc/Fulbright Scholar at the University of Maryland in Baltimore, USA. His PhD was at Institute for Genetics and Molecular Medicine, University of Edinburgh and he studied Pharmacy as an undergraduate at Cardiff University.

Dr Simon Rogers

Senior Lecturer, University of Glasgow

Simon is a senior lecturer in the School of Computing Science at the University of Glasgow, where he has had a permanent post since 2009. He is also an affiliate member of Glasgow Polyomics. His current research involves the development and use of Machine Learning approaches to tackle problems in metabolomics. Most recently he has led the development of MS2LDA, a topic modelling algorithm for extracting substructure 'topics' from MS/MS data. He has a background in applying Machine Learning approaches to -omics data and, as well as metabolomics, has published methods for proteomics and transcriptomics, and has worked in this area since completing his PhD ('Machine Learning Techniques for Microarray Analysis') at the University of Bristol. With Prof. Mark Girolami, he is the co-author of an introductory Machine Learning textbook 'A first course

Dr Wendy Russell

Gut Heath Theme Leader, Rowett Institute of Nutrition and Health, University of Aberdeen

Wendy is a chemist specialised in molecular nutrition researching the complex interplay of diet and health. Her research aims to establish the metabolic phenotype for different population groups and the impact of dietary modulation. She has conducted several human dietary interventions involving modulation of food components to understand their role in preventing disorders such as cardiovascular disease, type 2 diabetes and cancer. Wendy has funding from the Scottish Government Strategic Research Programme to investigate opertunities for novel crop production, particulary in protein provision for the future and in the exploitation of underutilised species. Wendy also has current funding through an NIH (US) competitive grant to investigate the role of diet in cancer aetiology, a Leverhulme; Artist-in-Residence grant 'Imagining the Future Food System'and a CAPES (Brazil) funded research programme on reformulation with sustainable and healthy food ingredients. Wendy is an editor for Food and Nutrition Science and chairs ILSI expert groups on 'nutritional management of postprandial glycaemia' and 'efficacy of intervention in those with metabolic syndrome.

Dr David Watson

Reader, University of Strathclyde

David Watson has worked with chromatographic and mass spectrometry techniques for 38 years. Interested in clinical and model systems for studying metabolic responses. Local organiser and chair of the 2013 Metabolomics Society Conference in Glasgow. Also interested in the biological properties of propolis and organised the first international conference on propolis in Glasgow in 2016. Dr Watson has supervised 44 PhD students to completion. He is the author of two textbooks on Pharmaceutical Analysis, which has been translated into six languages, and Pharmaceutical Chemistry. Published 290 papers and reviews. H index 40. External examiner for 22 PhD students in the last fifteen years. External examiner for the MPharm and Pharmaceutical Sciences Courses at John Moore's University 2010-2013 and currently the MSc in Drug Discovery at the University of Sunderland. On the editorial boards of Phytochemical Analysis and Current Metabolomics.

Dr Jimi Wills

IGMM Mass Spectrometry Laboratory Manager, University of Edinburgh

Jimi started off in the University of Glasgow, getting both his undergrad BSc in Molecular and Cellular Biology in 2001, and his PhD in the crossover between anatomy, molecular genetics and mass-spec-based proteomics in 2006. He spent a year on a stem-cell commercialisation project at Glasgow Royal Infirmary before joining Juri Rappsilber in Edinburgh University, with whom he worked for 7 years. During this time he became very familiar with Thermo Orbitrap systems and their data, along with a bunch of different LC systems. Throughout his career, Jimi has answered problems of data volume, repetition and human error with computer programming, a skill he's been developing since he was 5 years old. Jimi took up his current post in spring of 2014 and now coordinates protein, metabolite, lipid and other experiments on two QExactives in an institute of 500 researchers.

Dr Simon Young

Research Fellow, University of St. Andrews

Simon's principal research focus is the study of lipid metabolism in *Trypanosoma brucei*, the causative agent of Human African Trypanosomiasis, a neglected tropical disease of sub-Saharan Africa. This disease is fatal if not treated and current therapies are largely ineffective, toxic and out-dated, thus there is a significant demand to identify new drug targets and inhibitory compounds for these protozoan parasites. He obtained his B.Sc. and Ph.D. at the University of Glasgow and even at that stage was involved with this tropical disease, spending significant time as a visiting scientist in Kenya. Since then Simon has spent his academic career entirely in Scotland, at the Universities of Edinburgh, Dundee and now St. Andrews. In his research I commonly uses mass spectrometry as a tool to phenotype the effect of genetic modifications and chemical treatments on metabolic processes in these protozoan parasites. Having a range of mass spectrometric configurations at my disposal has aided a number of collaborations analysing the lipids and metabolites of a wide variety of organisms. Often this illuminates how organisms fundamentally adapt their lipid metabolism and membrane composition to cope with genetic or chemical interferences and physical stresses.

Dr Kerstin Ziegler

Postdoctoral Research Fellow, University of the Highlands and Islands

Kerstin studied undergraduate Chemistry at the University of Bonn and then specialised in Food Chemistry at the Technical University of Berlin. She then obtained a Master's degree in Bioscience from the University of Leeds and went on to study absorption and metabolism of bioactive food compounds in the group of Prof Gary Williamson for her PhD. Since 2015 she has held the position of Postdoctoral Research Fellow in Lipidomics at University of the Highlands and Islands where she is working on the analysis of lipid mediators, specifically eicosanoids.

Industry Speaker Biographies

Dr Stephen Ayris
Sciex

Steve started academic life at the Durham University completing his undergraduate degree and then on to University of Birmingham to complete his PhD. After which he joined the Forensic Science Service as mass spectrometry specialist (when mass specs were the size of Noah's Ark) then on to be a mass spectrometry instructor at Thermo's training center. Then he found his true calling when the dark side of sales knocked at his door and has spent the past 12 years to where he finds himself now as the business manager of the UK, Ireland and Nordics for SCIEX.

Dr Lidia Jackson
Principal Applications Chemist, Waters

Lidia Jackson is a Principal Applications Chemist working in the Waters Applications Laboratory in Wilmslow, UK. She has recently moved to the Northern European Demo Lab where she is responsible for developing and demonstrating solutions for high resolution mass spectrometry analysis of small molecules. Prior to that, she has spent six years in the European Applications Lab working across a range of large and small molecules applications. She was specifically focusing on lipidomics, metabolomics, metabolite identification, impurity profiling, accurate mass and toxicology screening as well as biopharmaceutical analysis. Prior to joining Waters, Lidia completed a PhD in the study of metallodrug protein binding by LC-MS at the University of Sheffield, UK.

Dr Anas Kamleh
Applications Specialist, Thermo Fisher Scientific

Anas Kamleh obtained his first degree in Pharmacy (2001) from Damascus University with first class honours, followed by a postgraduate diploma (PGDip) in qualifications of medicinal products (2002). In 2006, he obtained a scholarship for a PhD in analytical Chemistry at University of Strathclyde which was concluded in 2010. In 2009, Anas moved to work as a research assistant at Imperial College London at the department of Surgery and Cancer and upon graduating his PhD, he was promoted to the position of a research associate. He was part of the ENVIROGENOMARKER consortium that applied a multi-omics approach for mechanistic as well as biomarker discovery in cancer. In 2012, he started a postdoctoral research position at the Karolinska Insitutet in the Wheelock lab. The position was a continuation for his previous expertise focusing on biomarker discovery in cardiovascular diseases. In 2015, he became an applications Specialist NPI- Omics and LSMS support and training specialists at Thermo Fisher Scientific where he is training scientists for making the most out of Orbitrap technology.

Dr Anthony Sullivan

Mass Spectrometry Product Specialist, Agilent Technologies

Anthony Sullivan is a Mass Spectrometry Product Specialist at Agilent Technologies who serves the UK / Nordic region in Academia. Anthony has 20 years of experience in the field of Mass Spectrometry, with a Ph.D. from the Gaskell Group at the University of Manchester and subsequent work experience in the UK and USA, including Ciba Specialty Chemicals and the Windber Research Institute. Anthony's contributions to the Mass Spectrometry community include founding the London Biological Mass Spectrometry Discussion Group, and he also serves as Meetings Secretary for the British Mass Spectrometry Society.

Dr Christopher Titman

Senior Technical Specialist, LCMS & Life Science, Shimadzu UK Ltd

Chris has provided scientific support for mass spectrometry at Shimadzu for almost 9 years where his role has always involved customer support, training and method development. Moreover, he has been directly involved in the development of new applications for mass spectrometry for over 10 years. His career began in protein science obtaining a Biochemistry degree from Imperial College London in 2001 before completing a Ph.D. in structural enzymology at the University of Cambridge. It was in Cambridge, while responsible for the development of LCMS methods for metabolomics with Jules Griffin, that his enthusiasm for training was enhanced through collaborative projects and support of students within the laboratory.

Poster Titles

Poster Board A1
Comparing the effects of different cultivation practices on the metabolite composition of cereal crops
T. Shepherd, G. Dobson, D. McRae, J. Sungurtas, S. Pont, R. Palau, C. Alexander, S. Verrall, D. Stewart, L. Shepherd

Poster Board A2
The wider application and adaptation of a quantitative assay developed to assess paracetamol metabolism
N.Z. Homer, K. Sooy, Y. Jin, R. Mitchell, M. Eddleston, J. Dear, K. Morgan, L.J. Nelson, M.J. Hughes, R. Andrew

Poster Board A3
Development of an LC-MS/MS method for analysis of estrogen and its metabolites in human plasma
N. Denver, N.Z.M. Homer, S. Khan, R. Andrew, S. Fowles, M.R. MacLean

Poster Board A4
Determining the role of altered sphingolipid metabolism in oncogene-induced senescence
Flora L. Dix, Andrea Quintanilla, Mary K. Doherty, Seshu R. Tammireddy, Joy Edwards-Hicks, Rachel White, Andrew J. Finch, Phillip D. Whitfield, Juan-Carlos Acosta

Poster Board A5
Energetic shortfall during myc-induced apoptosis
Huizhong Su, Joy Edwards-Hicks, Jimi Wills, Andrew J. Finch

Poster Board A6
A novel strategy for absolute quantification of twenty amino acids in serum samples by post-analysis of LC-MS based untargeted metabolomics data
Tong Zhang, Oliver Maddocks

Poster Board A7
Exploring the fragmentome with unsupervised clustering and topic models
Justin J. J. van der Hooft, Joe Wandy, Sandosh Padmanabhan, Rónán Daly, Michael P. Barrett, Karl E.V. Burgess, Simon Rogers

Poster Board A8
Assessing the limit of quantification in the analysis of lipid mediators by LC-MS/MS
Kerstin Ziegler, Phillip D. Whitfield

Poster Board A9
Eicosanoid profiling: A novel tool for assessing nanoparticle toxicity
Kerstin Ziegler, Elizabeth Garrison, Benjamin H. Maskrey, Sean Semple, Mark R. Miller, Rodger Duffin, Janet Adamson, Ian L. Megson, Phillip D. Whitfield

Poster Board A10
Surviving starvation: Lipidomic analysis of algae under nutrient deprivation
Seshu R. Tammireddy, Mary K. Doherty, Sarah F. Martin, Elaine Salvo-Chirnside, Thierry Le Bihan, Phillip D. Whifield

Poster Board A11
Hair or hair follicle, the potential metabolic biomarker in the future?
Wenjuan Cong, Tong Zhang, Jeff Evans, Fiona Thomson

Poster Board A12
Mapping metabolism in the parasite Trypanosoma brucei using U-13C labelled amino acids and LC-MS
Katharina Johnston, Dong-Hyun Kim, Michael P. Barrett, Fiona Achcar

Poster Board A13
The effects of exposure of UV light on the urinary metabolome
Ali Muhsen Ali, David Watson

Poster Board A14
Comparison of the metabolism of mephedrone in cultured and in freshly isolated primary rat hepatocytes
Ibrahim Alanazi, M. Helen Grant, David Watson, Catherine Henderson

Poster Board A15
The effects of cis platin on the metabolome of sensitive and resistant ovarian cancer cells
Sanad Alonezi, David Watson

Poster Board A16
Metabolomic changes in pediatrics with Crohn's Disease
Adel Alghamdi, Vaios Svolos, Konstantinos Gerasimidis, David Watson

Poster Board A17
Metabolomics profiling of nitric oxide donor impact on the smooth muscle cells
Abdulwahab Alamri, David Watson

Poster Board A18
Metabolomics flux of prostate cancer using sphingosine kinase inhibitors by LC-MS
Mohammad Alrofaidi, David Watson, Nigel Pyne, Susan Pyne

Poster Board A19
Metabolomics in metabolic disease
P. David Eckersall

Poster Board A20
Understanding cholesterol metabolism in pancreatic cancer
Grace McGregor, Sergey Tumanov, Jurre Kamphorst, Owen Sansom

Poster Board A21
Triglycerides maintain membrane saturation
Sergey Tumanov, Daniel Ackerman, Bo Qiu, Celeste Simon, Jurre Kamphorst

Poster Board A22
Can 1H NMR spectroscopy predict incident heart failure in the elderly?
Naomi Rankin, Christian Delles, Charles Boachie, Alex McConnachie, Ian Ford, Antti Kangas, Pasi Soininen, Peter Wurtz, Mika Ala-Korpela, Paul Welsh and Naveed Sattar

Industry Poster Titles

Industry Poster 1 - Thermo Fisher Scientific
Increased Metabolome Identification Coverage Using Optimized LC MS-MS Condition on a Tribrid Orbitrap Mass Spectrometer
Reiko Kiyonami, Claire Dauly, Ralf Tautenhahn, David Peak, Ken Miller

Industry Poster 2 - Thermo Fisher Scientific
Discovering Potential Diabetic Lipid Biomarkers Using HRAM LC-MS-MS Approach on a Hybrid Quadrupole-High Field Orbitrap Mass
Reiko Kiyonami, Elena Sokol, David Peake and Ken Miller

Industry Poster 3 - Thermo Fisher Scientific
The ETD-Like Fragmentation for Small Molecules
Romain Huguet, Tim Stratton, Chad Weisbrodt, Mark Berhow

Industry Poster 4 - Waters
Utilising an IMS-DIA-MS Workflow to Characterise and Quantify the Obesity or Diabetes lipidome in Human Plasma
Lee A. Gethings. LeRoy B. Martin, Johannes P.C. Vissers, Jose Castro-Perez, James I. Langridge

Industry Poster 5 - Waters
Metabolomic Workflow Utilising Rapid Microbore Metabolic Processing (Rammp) in Conjunction with a Novel Scanning Quadrupole DIA Method
Lee A. Gethings, Chris Hughes, Keith Richards, Mike Morris, Jason Wildgoose, Johannes P.C. Vissers, James Langridge

Industry Poster 6 - Waters

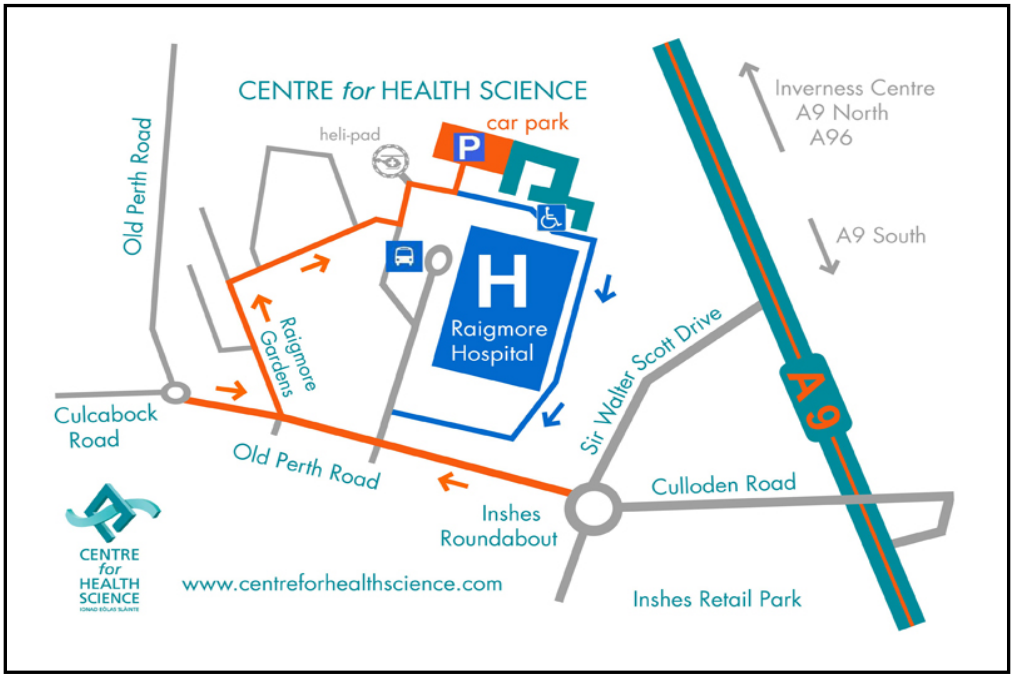
Automatic CCS and MS/MS Library Creation and Application for Large Scale Metabolic Profiling
Jonathan P. Williams, David Eatough, Lee A. Gethings, Christopher J. Hughes, Mark Towers, Leanne Nye, Steven Lai, Richard Tyldesley-Worster, Suraj Dhungana, Johannes P.C. Vissers

Industry Poster 7 - Shimadzu
Exploring Changes in Primary Metabolites in Alzheimer's Disease using Targeted LC-MS/MS
Nicola Gray, Stuart Snowden, Min Kim, Chris Titman, Cristina Legido-Quigley

Industry Poster 8 - Shimadzu
Mass Spectrometry-Based Metabolomics to Differentiate Beer Types
Shuichi Kawana, Takero Sakai, Yusuke Takemori, Daichi Yukihira, Tsuyoshi Nakanishi

Venue - Centre for Health Science

http://www.centreforhealthscience.com/



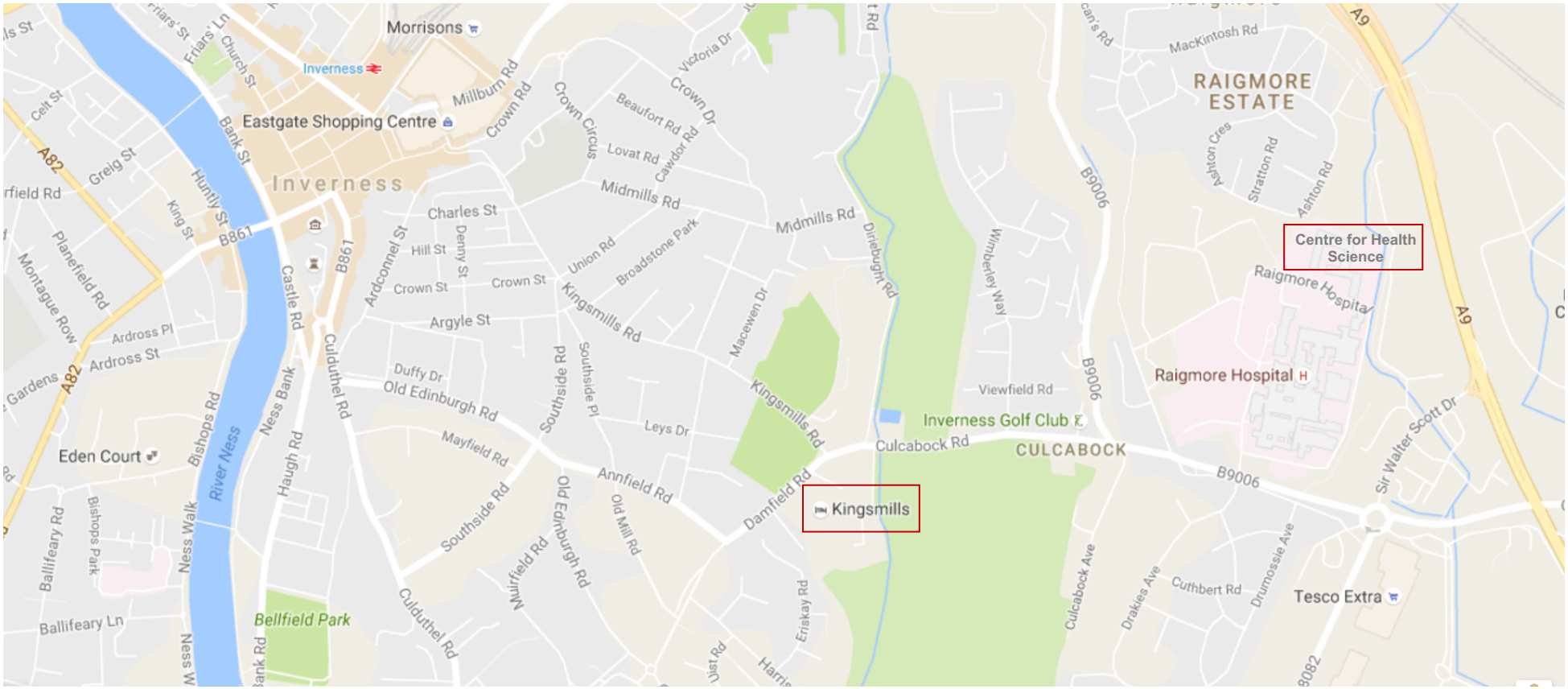
The Centre for Health Science is located behind Raigmore Hospital

Evening Event

The Highland Council is hosting a Civic Dinner for delegates of the Scottish Metabolomics Network Meeting

Start: 19:00-19:30

Venue: The Kingsmills Hotel, Culcabock Road, Inverness IV2 3LP



Acknowledgments

There are a number of people that we would like to thank in assisting us with the organisation of the Scottish Metabolomics Network Meeting 2016. In particular, our colleagues at the University of the Highlands and Islands, Kerstin Ziegler, Seshu Tammireddy, Janet Adamson, Laura Chisholm and Tim Miles as well as Adam Brown of Robertson Facilities Management at the Centre for Health Science.

We would also like to thank Karl Burgess and Naomi Rankin at the University of Glasgow for their input along with the organising committee from last year's meeting at the University of Edinburgh, Ruth Andrew, Andy Finch and Natalie Homer. Finally, a special thanks to Danielle Marlow (University of Edinburgh) for her considerable help.

Phillip Whitfield and Mary Doherty
University of the Highlands and Islands