12th December 2016

- Special issue on the Scottish Metabolomics Annual Meeting

**Overview (from Karl Burgess and Naomi Rankin)**

An exciting year for the Scottish Metabolomics Network has culminated in a wonderfully successful second annual conference, held at the University of the Highlands and Islands’ Centre for Health Science in Inverness.

Attendance was again exceptional, with more than 80 delegates braving the cold weather to visit Inverness in November. Again, Karl was struck by the collegiate atmosphere and the lack of the hierarchies that mar other conferences. Karl’s original model for the SMN was to make it more like the Proteomics Methods Forum (PMF), sort of a national lab meeting, where metabolomics groups could present some of their work, students could have the opportunity to present their work in a supportive environment. While we aren’t all as technology focused as those in the PMF, he thinks we have the same feeling of community.

Karl was proud to announce our official affiliate status with the Metabolomics Society, organised by Reza Salek and Merlijn van Rijswijk and ratified by Ute Roessner. This necessitated a more formal structure than our previous free-for-all, with myself as Chair and Metabolomics Society Liaison, Andy Finch as Secretary and Ruth Andrew as Treasurer. Additionally, we now have a website: scottishmetabolomics.net. We are excited to see where we progress in future.
We would like to thank all the sponsors, without whom this meeting would not have been possible: Agilent Technologies, the Royal Society of Chemistry, Sciex, Shimadzu, SULSA, Thermo Scientific, Waters, Advion and Crawford Scientific. A special thank you to Anas Kamleh (Thermo Fisher Scientific), who updated us on the evolution of the Orbitrap since 2005, and introduced the Orbitrap Tribrid; Lidia Jackson (Waters), who demonstrated how ion mobility was helping to identify lipids in obesity and Diabetes; Anthony Sullivan (Agilent Technologies), who demonstrated how the Seahorse can be used in combination with MS based MRMs to better understand cell bioenergetics; Steve Ayris (Sciex), who introduced the Lipidyzer platform for the absolute quantification of over 1000 lipid molecular species by incorporating deuterated internal standards and finally to Christopher Titman (Shimadzu), for demonstrating the use of their targeted LC-MS method for investigating changes in primary metabolites in Alzheimer’s disease. Special thank you again to the Royal Society of Chemistry, Analytical Division, for sponsoring the prizes and congratulations to Joy Edwards-Hicks (University of Edinburgh) for winning the prize for best talk from an Early Career Researcher, Nina Denver (University of Glasgow) for winning People’s Choice award for her poster, Grace McGregor (Beatson Institute for Cancer Research) for winning the poster prize, Ali Muhsen Ali (University of Strathclyde) and Flora Dix (University of Edinburgh) for winning the runner up poster prizes. We are sure Councillor Helen Carmichael, the first female provost of Inverness and area would be impressed. Six of the 15 invited speakers were female (40%), reflecting the 38% female audience. Additionally about half the chairs and judges were female. We would also like to thank The Highland Council for hosting the Civic Dinner.

We would again like to thank Phil Whitfield and his team (Mary Doherty, Laura Chisholm, Tim Miles), his support from Adam Brown from Robertson's Facilities Management, and from the previous year’s inaugural conference organisers: Ruth Andrew, Natalie Homer, Andy Finch and Danielle Marlow. Everything looked relaxed and streamlined, and from previous conference organisation experience, Karl knows how stressful and difficult that is to achieve! We would also like to thank our keynote speaker, Matt Dalby, for an exciting look into the applications of metabolomics in cell engineering. The two previous years have presented a high bar for the Glasgow meeting (especially in inviting the Provost of Inverness to join us for dinner!). I hope we can live up to your expectations in 2017!
In the ‘Metabolomics in Biology’ sessions we had several great talks that highlighted the diversity of applications of metabolomics in Scotland. Wendy Russell (Rowett Institute, Aberdeen) began the session by discussing the use of targeted metabolomics to investigate the effect of different dietary interventions on the gut microbiome. She described how different diets affect the metabolic status of individuals and how certain crops can be more beneficial than others. On a related theme, Oliver Maddocks (University of Glasgow) gave us a fascinating insight into how dietary availability of amino acids (serine in this case) could impact upon tumour incidence - a serine-free diet in mice offered significant protection from cancer caused by discrete mutations. Oliver’s work suggests that dietary intervention could play a role in the treatment of certain cancers in the clinic - a very exciting prospect. Simon Young (University of St. Andrews) presented a study looking at the composition of the trypanosomal lysosome, with a long-term goal of generating agents that disrupt trypanosomal lysosome function and therefore viability. This organelle has not been well characterised thus far, mainly due to technical issues with its isolation - this is an area that Simon is optimising at the moment. Initial methods using a detergent that accumulates in the lysosome, allowing subsequent separation by density, have provided robust lysosomal purifications but more physiological methods are also in development.

On the second day, we heard Joy Edwards Hicks (IGMM, Edinburgh) talk about how the oncogene c-Myc leads to activation of the tumour suppressive p53 pathway. Joy revealed a critical role for ceramides in this process and has therefore been characterising these lipids and metabolic flux into them to try to understand this process - well done to Joy on winning the Early Career Researcher talk prize, sponsored by the Royal Society of Chemistry. We then heard from Will Allwood (James Hutton Institute) who gave us an overview of the versatile analytical techniques employed in their facility near Dundee: the main focus of the Institute is upon crops and bioavailability. The application that Will presented was a study of the presence of bitter metabolites in various feeds that led to different uptake by pigs - a good example of how metabolomics can yield insights with clear financial and health benefits. Rebecca Goss (St Andrews) closed the second ‘Metabolomics in Biology’ session. She presented a wonderful fusion of chemistry and genetics focussed upon development of generating new drugs (e.g. antibiotics). Rebecca’s lab have been...
generating novel precursors that can be incorporated into biosynthetic pathways in bacteria yielding complex molecules with a moiety that can be derivatised. This opens up exciting possibilities in the development of new drugs.

**Technical Sessions Overview (from Natalie Homer)**

In the ‘Pipelines and Workflows’ session the focus was on the importance of experimental approach and design. Dave Watson (Strathclyde University) described derivatisation strategies to enhance not only detection but also separation of compounds, in particular the power of the chemical nature of the derivative in improving resolution of the many hexose isomers found in urine.

Karl Burgess, from Glasgow Polyomics, gave a fascinating talk about cultural heritage. He described a clever analytical approach to detecting forgery of Robert Burns (1756-96) poetry by renowned forger Alexander Howland (‘Antique’) Smith from the 1880s. Using LESA of inks on manuscripts he exploited and identified differences in composition of inks from pre and post-industrial times. Gillian Mackay from the Beatson Institute for Cancer Research in Glasgow talked about untargeted metabolomics using Progenesis QI software, with the intention of identifying metabolites changed in cancers. Again, the importance of good separation of metabolites to aid in their identification was discussed and logical and systematic approach to sample analysis.

In the ‘Software and Bioinformatics’ session, Simon Rogers (Glasgow University), described MS2LDA, an unsupervised method of Tandem MS data analysis for untargeted metabolomics, inspired by text-mining. Simon deftly used ‘Hereford United’ in a text search to illustrate how a dataset can be interrogated and how this in turn can relate to fragment and neutral loss features in a typical tandem MS dataset. Jimi Wills (Edinburgh University) described in-house software that he has generated to improve upon what proprietary software packages can do. He illustrated the strength of custom-built tools for quantitative measurement in metabolic pathways.
Photographs:

1. Helen Carmichael (Provost and Leader of Inverness and Area) and Karl Burgess (Glasgow Polyomics), photograph courtesy of Matt Dalby.
2. Prize winners: Joy Edwards-Hicks (University of Edinburgh), Nina Denver (University of Glasgow), Grace McGregor (Beatson Institute for Cancer Research) and Flora Dix (University of Edinburgh), photograph courtesy of Seshu Temmireddy.
3. Wendy Russell (Rowett Institute, Aberdeen) and attendees, photograph courtesy of Karl Burgess
4. Ruth Andrew (University of Edinburgh), Nina Denver (University of Glasgow), Natalie Homer (University of Edinburgh), photograph courtesy of Oliver Maddocks.

If you have anything you want to add to the next edition of the newsletter please e-mail Naomi.rankin@glasgow.ac.uk.