



# Scottish Metabolomics Network Newsletter

16th of August 2018

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For twitter updates search for [#ScotMetNet](#)

## Scottish Metabolomics Network Symposium 2018 Advert (from Will Allwood and Jeffery Huang)

The next Scottish Metabolomics Symposium will be held at the **Discovery Point Exhibition Centre on Thursday the 1<sup>st</sup> and Friday the 2<sup>nd</sup> of November 2018**. More information can be found on the [SMN website \(events page\)](#). You can download a flyer to display in your workplace and a link to the Dundee and Angus Convention Bureau where you can get more information about Dundee as well as discounted rates for hotels and visitor attractions. Early Bird registration (£40) closes **19<sup>th</sup> September 2018** (Registration will be £60 after this date). Deadline for poster abstracts is the **19<sup>th</sup> September 2018** (note: abstracts will only be considered from authors who have registered for the SMN18).

Themes will be metabolomics technologies, cancer metabolomics, lipidomics, food and crop chemistry and nutrition and metabolomics in biomarker research. The evening drinks reception will be held on board the RSS Discovery followed by the conference dinner. Enquiries to [will.allwood@hutton.ac.uk](mailto:will.allwood@hutton.ac.uk) and [wtrcf.education@ed.ac.uk](mailto:wtrcf.education@ed.ac.uk)



This year we are delighted that [Dr. James MacRae](#) of the [London Metabolomics Network](#) will be attending the SMN 2018 meeting in November in Dundee. This is part of an ongoing initiative to build interactions between national and international Metabolomics groupings. We look forward to welcoming him and hearing his talk entitled “Lipid Metabolism in apicomplexan parasites: Routes for drug therapy?”



We look forward to welcoming you to Dundee. For updates follow [#ScotMetNet](#) on Twitter.

### Scottish Metabolomics Network Lab Visit Training Grants for Early Career Researchers 2018

We are pleased to be able to offer a new initiative through the SMN: the **SMN Lab Visit Training Grants for Early Career Researchers**. We are now seeking to award 3 or 4 Early Career Researchers from our network laboratories a grant to visit and train in another network lab. Applications for these grants are now invited with a **Deadline of 29th September 2018**, and awards will be made at the Annual Symposium in November 2018 in Dundee. An application form, with more details, can be downloaded on the [events page](#) of the SMN website.

### Laboratory of the Quarter: Glasgow Polyomics Facility, University of Glasgow (from Karl Burgess)

Glasgow Polyomics is a multiomics facility based on the Garscube campus of the University of Glasgow. Our team aims to provide a comprehensive coverage of 'omics experiments from concept design through to data interpretation and publication. Born as the Sir Henry Wellcome Functional Genomics Centre, Glasgow Polyomics expanded in 2008 to include proteomics and metabolomics capabilities to a wide range of academic and industrial customers.



The metabolomics team has recently benefited from grants from SULSA and Wellcome Institutional Strategic Support Fund, allowing the expansion to a team of seven members, assisted by the Polyomics administrative team. Headed by Dr Karl Burgess, the expert team is composed of two technicians, two mass spectrometry specialists/technologists and two bioinformaticians/data analysts allowing us to call on a wide body of knowledge and experience. We have experience with a diverse range of sample types and help users design and plan experiments, producing high quality data along with biochemical interpretation leading to high impact publications. We have been involved in a large number of successful grant applications, many with industrial partners, and are happy to discuss and participate in any future applications requiring metabolomics input.

Our close collaboration with Thermo Scientific has led to us focusing on Orbitrap mass spectrometers for our metabolomics platform. Our current instrument portfolio includes an Exactive, Q-Exactive and Fusion (run in conjunction with the Wellcome Centre for Molecular Parasitology) allowing us to carry out experiments ranging from routine screening analysis to specific, targeted fragmentation identifications of novel components. We also have a Thermo ion trap GC-MS that is used for a variety of targeted work.

We routinely run untargeted metabolomics, focussing on small, polar metabolites and our standard analytical platforms are geared towards these types of analyses. We also have a range of targeted methods for specific classes of metabolites and expertise in isotope labelling analysis to further investigate changes discovered via untargeted analysis.



Interpretation of metabolomics data can be difficult, requiring knowledge of the instrumentation, bioinformatics and biochemical understanding to get the best from an experiment. We provide support for every aspect of metabolomics experiments and our metabolomics software pipeline, Polyomics integrated Metabolomics Pipeline (PiMP), provides an easy way to investigate LC-MS data in the context of biochemical pathways. We have in-house support in complex analyses from an advanced statistics team who can be involved in projects that require advanced statistics, such as data modelling and pattern matching.



For more high throughput users of the service, we also provide training and workshops in PiMP as well as running an “Intro to Omics” course for people that wish to know more about what each ‘omic can be used for.

Our overall goal is to provide a cutting-edge metabolomics service that goes beyond the running of samples and return of raw instrument data. We take pride in the relationships we have built with research groups both at Glasgow University and around the world. If you think metabolomics may aid your research but are unsure where to start, then please don't hesitate to get in touch <http://www.polyomics.gla.ac.uk/enquiry.php>

Some of our highlight papers include:

Newton, James, et al. "Minimally-destructive atmospheric ionisation mass spectrometry authenticates authorship of historical manuscripts." *Scientific reports* 8.1 (2018): 10944.

McMurray, Rebecca J., et al. "Nanoscale surfaces for the long-term maintenance of mesenchymal stem cell phenotype and multipotency." *Nature materials* 10.8 (2011): 637.

Creek, Darren J., et al. "Toward global metabolomics analysis with hydrophilic interaction liquid chromatography-mass spectrometry: improved metabolite identification by retention time prediction." *Analytical chemistry* 83.22 (2011): 8703-8710.

Connolly, James PR, et al. "The host metabolite D-serine contributes to bacterial niche specificity through gene selection." *The ISME journal* 9.4 (2015): 1039.

Haggarty, Jennifer, et al. "Serially coupling hydrophobic interaction and reversed-phase chromatography with simultaneous gradients provides greater coverage of the metabolome." *Metabolomics* 11.5 (2015): 1465-1470.

## Core Technologies in Life Sciences (CTLS) Conference 2018 in Ghent (from Natalie Homer)



## Core TECHNOLOGIES FOR LIFE Sciences

The aim of the Core Technologies for Life Sciences (CTLS) is to '***bring together scientists, technical and administrative staff working in or in close association with core facilities, research infrastructures and shared resource laboratories in life sciences and biomedicine***'. The third biennial CTLS conference was held from 1<sup>st</sup>-4<sup>th</sup> July 2018 in Ghent at the Flanders Institute of Biotechnology, VIB, which is a non-profit research institute in Belgium.

There were plenary and parallel sessions on topics that were of interest to all types of cores, regardless of scientific discipline. These included benchmarking, exchanges on best practice, emerging technologies, finances and contracts, training for core staff and supporting career development at all stages. A number of software packages that lessen the load for facility management were discussed and showcased by vendors where the capabilities of these packages are a huge jump from self-made processes and procedures developed in isolation.

Discussions revealed that a greater understanding of what is involved in managing and working within a core facility is needed. Retention of staff and their knowledge within a facility is essential for efficient operation and that can only be achieved if there is career development for core scientists. There is a need for ongoing training of core staff for efficient management and operation and a Training Working Group of the CTLS has been established to address this.

There was emphasis placed on the importance of networking and learning from others in terms of operation and management but also facilitating and promoting access to cores. A number of European networks and collaborations presented findings in posters and sessions such as EULIFE and networks such as CORBEL ([www.corbel-project.eu](http://www.corbel-project.eu)) and NEUBIAS ([www.neubias.org](http://www.neubias.org)).

In general CTLS2018 illustrated that those that offer a shared resource, a facility or support research within an institute or university all encounter similar problems and that working together to improve operations and management will only improve cores and add to the scientific outputs of institutes and universities.



## Cold Spring Harbor Laboratory Metabolomics Course (from David Sumpton)

Since the Cold Spring Harbor laboratory (CSHL) metabolomics course was founded in 2016, members of the metabolomics facility at Beatson Institute have assisted in its organisation and delivery. In June, David Sumpton from the facility returned for his second year.

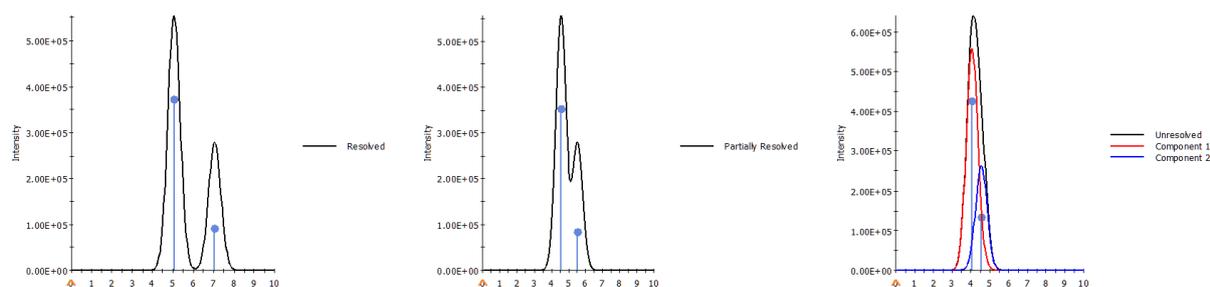
The course is very technology driven, through a close collaboration with Agilent Technologies and Thermo Fisher Scientific, with a pop-up mass spectrometry lab assembled over a matter of weeks. A wide range of high-end instrumentation is made available for the students, from LC and GC triple quads, LC- time of flight (ToF) and LC-Orbitrap instrumentation. Over a period of two weeks, the students learn both the fundamental theory and application of these different GC/LC-MS methodologies to answer biological questions. Key concepts are further emphasised through practical sessions with considerable amounts of hands-on time. As part of the broader programme, students also hear talks from more than a dozen invited speakers working in the metabolism field. Each speaker gives two presentations, an informal and often interactive chalk talk underlining the main experimental tools they employ in their own research and a more formal big picture scientific talk summarising their work. Speakers this year included Matthew Vander Heiden (Massachusetts Institute of Technology), Teresa Fan (University of Kentucky College of Medicine), our own Eyal Gottlieb (Cancer Research UK, Beatson Institute, Glasgow), a founding instructor of the course, and Steve Gross (Weill Cornell Medical College, New York).

The whole process is extremely challenging but also very rewarding. The Cold Spring Harbor campus is beautiful in summer. The isolation and intense timetable leads to a fully emergence experience, one in which we, along with the students, always learn a great deal.



## Notes from our Sponsors: Chromatographic Deconvolution (from John Moncur, SpectralWorks Ltd.)

GC-MS and LC-MS play an important part in the metabolomics workflow. Deriving features from these analytical techniques is a significant part of this workflow. Peak overlapping or partial co-elution is a common problem in any chromatographic separation technique. Where a detector which produces spectral characteristics is used, such as a mass spectrometer, the deconvolution of partially overlapping peaks can be achieved without any assumptions being made regarding the peak shape or underlying spectra of the individual components. Figure 1 shows the purpose of chromatographic deconvolution as the resolution between two components is reduced. From fully resolved to unresolved, AnalyzerPro is able to determine the two components in each case.



The benefits of deconvolution can be realised in two ways. The number of features determined in samples may be increased and/or the required chromatographic resolution may be reduced. The effect of the latter is to help reduce analysis time.

Deconvolution brings with it the question of how many data points need to be acquired across a peak? If we reduce the issues of peak fronting and tailing and take the peak width at Full Width Half Maximum (FWHM), typically 8 to 10 sample points would be expected in order to be able to reproducibly generate peak data. Even in the simplest case of partial co-elution, a sampling rate of 20 - 25 data points would not be unreasonable. The closer that the co-eluting components are together, then the more data points are required to generate reliable deconvoluted peak data.

Chromatographic peak deconvolution is very effective at determining multiple components in your samples.

### Scottish Metabolomics Network Papers

- AlRabiah, H., Allwood, J.W., Correa, E., Xu, Y., Goodacre, R. (2018). [pH plays a role in the mode of action of trimethoprim on Escherichia coli](#). *PloS one*, 13 (7). 10.1371/journal.pone.0200272
- Foito, A., Stewart, D. (2018). Metabolomics: [A high-throughput screen for biochemical and bioactivity diversity in plants and crops](#). *Current Pharmaceutical Design*. DOI: 10.2174/1381612824666180515125926
- Logie, L., Lees, Z., Allwood, J.W., McDougall, G., Beall, C., Rena, G. (2018). [Regulation of hepatic glucose production and AMPK by AICAR but not metformin depends on drug uptake through the equilibrative nucleoside transporter 1 \(ENT1\)](#). *Diabetes, Obesity and Metabolism*, pp 1-11. DOI:10.1111/dom.13455
- Newton, J, Burgess K et al. (2018). [Minimally-destructive atmospheric ionisation mass spectrometry authenticates authorship of historical manuscripts](#). *Scientific reports*, 8, pp.10944. DOI:10.1038/s41598-018-28810-2

## Awarded PhD studentships and grants

- **Promovendus - Eurolife Consortium (approx. £120k): 2018 -2022**
  - Joint PhD Studentship University of Leiden and University of Edinburgh (6 months secondment at University of Edinburgh) “Relieving head pain through modulation of the stress system” (van den Maagdenberg AMJM, Tolner EA, Andrew R, Mijer O)

## Metabolomics (and other) Conferences and workshops (in date order)

- [Androgens 2018 Meeting, 3<sup>rd</sup> - 5<sup>th</sup> September 2018.](#)
  - The University of Edinburgh, Edinburgh Medical School: Clinical Sciences
  - Registration open till 31<sup>st</sup> August 2018.
- [Glasgow Polyomics: Introduction to Python for Biologists, 3<sup>rd</sup> - 7<sup>th</sup> September 2018.](#)
  - University of Glasgow, Computer Cluster 515, West Medical Building, Glasgow.
  - Registration via enquiry form on website.
- [Glasgow Polyomics: An Introduction to Omics, 11<sup>th</sup>-12<sup>th</sup> September 2018.](#)
  - University of Glasgow, Jura Lab, Library, Main Campus, Glasgow
  - Registration via enquiry form on website.
- [Introduction to Metabolomics for the Microbiologist, 19<sup>th</sup>-21<sup>st</sup> September 2018.](#)
  - University of Birmingham, Birmingham Metabolomics Training Centre, Birmingham.
  - PhD students and post-doctoral researchers.
- [Introduction to Metabolomics for the Environmental Scientist, 27<sup>th</sup>-28<sup>th</sup> September 2018.](#)
  - University of Birmingham, Birmingham Metabolomics Training Centre, Birmingham.
  - Individuals with no previous experience of metabolomics.
- [Glasgow Polyomics: Metabolomics Data Analysis Course, 22<sup>nd</sup> -23<sup>rd</sup> October 2018.](#)
  - University of Glasgow, Jura Lab, Library, Main Campus, Glasgow
  - Registration via enquiry form on website.
- [Introduction to Metabolomics for the Clinical Scientist, 22<sup>nd</sup> October 2018.](#)
  - University of Birmingham, Birmingham Metabolomics Training Centre, Birmingham.
  - Individuals with no previous experience of metabolomics.
- [Scottish Metabolomics Network Symposium, 1<sup>st</sup> and 2<sup>nd</sup> of November 2018.](#)

- Discovery Point Exhibition Centre, Dundee, registration now open; Early Bird Registration (£40), closes 19<sup>th</sup> September 2018 (will be £60 after this date). **Lab Visiting Training Grants available (Deadline 29<sup>th</sup> September 2018)**
- [Metabolomics with the Q-Exactive, 19<sup>th</sup>-21<sup>st</sup> November 2018.](#)
  - University of Birmingham, Birmingham Metabolomics Training Centre, Birmingham.
  - Individuals with minimal experience of applying LC=MS in metabolomics studies.
- [Metabolite identification with the Q-Exactive and LTQ Orbitrap, 22<sup>nd</sup> -23<sup>rd</sup> November 2018.](#)
  - University of Birmingham, Birmingham Metabolomics Training Centre, Birmingham.
  - PhD students and post-doctoral researchers.
- [44<sup>th</sup> Adipose Tissue Discussion Group - Early Career Researcher Workshop, 6<sup>th</sup> December 2018.](#)
  - Queens Medical Research Institute, Edinburgh
- [44<sup>th</sup> Adipose Tissue Discussion Group Meeting, 7<sup>th</sup> December 2018.](#)
  - Informatics Forum, University of Edinburgh, George Square, Edinburgh.
  - Speakers include within other Profs Frederick Karpe (Oxford University) and Jimmy Bell (Imperial College). Further information can be obtained from [Nik.Morton@ed.ac.uk](mailto:Nik.Morton@ed.ac.uk), [rsemple@exseed.ed.ac.uk](mailto:rsemple@exseed.ed.ac.uk)
- [2019 Challenges in Analysis of Complex Natural Mixtures- Faraday Discussion, 13<sup>th</sup>-15<sup>th</sup> May 2019.](#)
  - Edinburgh, United Kingdom. Deadline Poster Abstracts, 4<sup>th</sup> March 2019.

## Webinars

New:

- [Agilent: On-going Omics seminar series](#)
  - A good resource to keep up with analytical developments in different laboratories around the world.
  - Webinars are available on demand but also as power point slides.
- [Metabolomics: Understanding Metabolism in the 21<sup>st</sup> Century.](#)
  - Course Length: 4 weeks (~3h per week)
  - 2018 Course Dates: Free course - Available now!
  - Recommended Level: Individuals with no previous experience of metabolomics.
- [Metabolomics Data Processing and Data Analysis.](#)
  - Course Length: 4 weeks (~4 hours per week).

- 2018 Course Dates: 8<sup>th</sup> October - 2<sup>nd</sup> November 2018.
- Recommended Level: MSc and PhD students in the early stats of analysing metabolomics data.
- [SCIEX: Innovation Advisory Board](#): a series of “lightening talks”
  - SCIEX account necessary
  - An Infusion “Shotgun” Approach for High-Throughput Untargeted Metabolomics by Marialuce Maldini
- [SCIEX: The Proteome: Composition and Organization](#)
  - 40 min video watch on demand

#### On Demand (Old):

- [Biomarker Discovery: SWATH Enabled- Metabolomics Differentiates Known Disease Classifications of Prostate Cancer](#)
  - 30 minute video, watch anytime
- [High Resolution Mass Spec Performance Without the Complexity](#)
  - Info-kit available upon registration
- [High-Throughput Proteomics Applications to Solve Major Biological Problems Around the Metabolic Network](#)
  - Webinar available upon registration
- [Protein Social Networks Studied By SWATH® Acquisition](#)
  - Webinar available upon registration

#### Further Announcements

- The [Metabolomics Society](#) Board has posted proposed amendments to the Society Bylaws for review and comment which can be found [here](#). Member comments are being solicited for 30 days before any further action is taken. Comments can be send to [secretary@metabolomicssociety.org](mailto:secretary@metabolomicssociety.org)

#### Vacancies

- [Anatune GC-MS Support Engineer](#), UK based, closing date 17<sup>th</sup> August 2018.
- CrawfordScientific Training & Technical Consultant, UK based, closing date 31<sup>st</sup> August 2018.
  - For further information please contact the Technical Services Manager Claire Paterson [claire@crowfordscientific.com](mailto:claire@crowfordscientific.com) (pdf document)
- [Sciex Support Specialist](#), open position, based in Warrington, UK
  - Small molecule analysis using QTraps and Q-ToFs for customer demos and onsite training

## Acknowledgement

Thank you to all the contributors and Naomi Rankin for help and advice. If you have anything you want to add to the next edition of the newsletter, please e-mail Sabine.Freitag@hutton.ac.uk.

### Photographs:

1. Dr James MacRae (photography courtesy of the Francis Crick Institute/Dave Guttridge)
2. Photograph of the RRS Discovery and the Discovery Point Exhibition Centre (<http://www.rrsdiscovery.com>)
3. Photograph of the Wolfson Wohl Cancer Research Centre where Glasgow Polyomics is situated (photograph courtesy of James Houghton)
4. Erin Manson and Suzanne McGill working at the Thermo Orbitrap Fusion Mass Spectrometer (photograph courtesy of James Houghton)
5. Isabel Vincent (left) taking a customer through her data (photograph courtesy of James Houghton)
6. Core Technologies in Life Science Logo ([www.ctls-org.eu](http://www.ctls-org.eu))
7. Natalie Homer presenting at the “Emerging Model Systems” session as part of the CLTS conference in Ghent (photograph courtesy of Valentina Adami, University of Trento, Italy)
8. Photograph of participants of the 2018 CSHL metabolomics course. Bottom row, course instructors: Justin Cross, Memorial Sloan Kettering Cancer Center. Amy Caudy, The Donnelly Centre, University of Toronto, Canada and Adam Rosebrock, Stony Brook School of Medicine, State University of New York. David Sumpton, Beatson Institute metabolomics facility (third from the right, on the backrow) “Cold Spring Harbor Laboratory Meetings & Courses Program” - official course photo)
9. Deconvolution of resolved, partially resolved and unresolved components. (courtesy of John Moncur, SpectralWorks, Ltd.)