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MetaboNews is a monthly newsletter published in partnership between The Metabolomics Innovation Centre (TMIC) and Metabolomics Society.

Welcome to the April 2018 issue of MetaboNews!

We are excited to bring you MetaboNews in a new media-rich format that we hope will bring a new level of engagement to all our loyal subscribers. The format is designed to be interactive, current, and provide a renewed outlet for industry news, columns and opinion pieces, interviews, training opportunities/events, jobs, and collaborative opportunities! We would like to welcome all members of the international metabolomics community, and those with an interest in the discipline, to get involved in *your* community and industry newsletter. So please do connect with us with any feedback, ideas and input you may have.

Metabolomics Society News

Register today for Metabolomics 2018!

The 14th Annual Conference of the Metabolomics Society will be held in Seattle, Washington, USA, on June 24-28, 2018. The Society's annual conference consistently features the latest and greatest advances in metabolomics science. In 2018, we converge in Seattle, a world-class metropolis set within the beautiful, natural surroundings of the Pacific Northwest.

Make sure to register now on our website:
http://metabolomics2018.org/registration

Workshops are now posted and available for signup as part of the Registration process. This year we will hold 15 workshops, including a Novice Track that includes Experimental Design, Mass Spectrometry, Statistical and Pathway Analysis and a Career Workshop. A broad range of more advanced workshops will cover areas such as Precision Medicine, Advanced Visualization, Metabolite Identification, QA/QC, Advanced Statistical Methods, Analysis Workflows, and many more. Several of these workshops include hands on activities. Space is limited in some workshops, so sign up early!

Student Housing Option - Now Available

Designed for students in search of a low-cost housing alternative, attendees can stay in a student dorm at the University of Washington. Click here for details. There are a limited number of rooms available at UW, don't delay!
For information about all conference hotel options, please click here.

METABOLOMICS 2018
JUNE 24-28 SEATTLE, WASHINGTON
14th Annual Conference of the Metabolomics Society

Board of Directors

Jules Griffin
Metabolomics Society President

Words From the President

This month we have been going through the bylaws of the Society. What started as a simple task to tidy up a few loose ends morphed into an hour-long discussion of how the bylaws reflect the current working of the Society.

In part this reflects the growth of the society. As I have mentioned previously we have decided to split the Conference and Training Committee into a Conference committee and a Training committee to reflect the growth in activity of both committees.

We also tidied up the terms that Directors can serve. Directors can serve two terms each of two years but we have now clarified how long the Early-career Members Network (EMN) chair can be a board member (a year as the EMN chair and then they are eligible for election to the board of directors in their own right for two terms) and also what happens if a director is elected mid-term to an officer position (they could serve five years, three as a director and then two as an officer).

Perhaps though the most important changes have been how we allow the membership have a say in the bylaws and running of the society. We have updated the bylaws to ensure they are consistent with electronic voting and consultation. The reason for telling you all this is that you have a chance to review these bylaw changes.

Prior to the Board of Directors approving the bylaws we have to display all the proposed changes for all the membership to review so please take a moment to look over these bylaws. While they can be somewhat dry they show how the society is evolving and please let us know if you think we have got anything wrong!

Amongst our discussions for the March BoD's TC was a move to rolling membership to the society. Currently everyone is a member for a calendar year so whether you join on the 1st January of this year or you join on the 30th December in both cases membership comes to an end at midnight, 31st December for that year.

This has the rather unfavorable feature that come 1st January each year the Society looks rather devoid of members! The intention going forward, starting from the 1st January 2019 we will introduce rolling membership of the Society.

We hope this will encourage members to renew on a date that suits them without their membership lapsing, and if you are late you don't miss out on a month or two's membership as you do under our current system. We hope this provides a fairer system.

Members Corner

Early Career Network (EMN)

EMN Webinar Series – 2018

EMN webinar was held on February 14 2018. **Prof. Uwe Sauer** (ETH Zurich, Switzerland) discussed the use of metabolomics data on generating hypotheses on the regulation of microbial metabolism.
You can access the recorded videos of the past webinars on the Metabolomics Society website. Please stay tuned and look out for the next EMN webinar series session.

EMN webinar session 17 was held on March 26 2018.
Dr. Nathan Lewis (University of California San Diego) discussed how we can capture an accurate view of cell or tissue specific metabolism from an expression profile. For the April session **Dr. Oliver Fiehn** has been scheduled, stay tuned for details.

You can access the recorded videos of the past webinars on the Metabolomics Society website. Please stay tuned and look out for the next EMN webinar series session.

EMN travel grant 2018: Applications are now closed!

We have received over 30 applications and are looking forward to announcing the winners after the evaluation. Winners will be announced in April on the Twitter, Facebook and the Metabolomics Society website. Selected abstracts and conference reports will be published in the MetaboNews/Metabolomics Society website.

New to metabolomics or stuck with a problem? We recommend Metabolomics wiki and Metabolomics Forum. Follow us on Twitter (@MetabolomicsSoc) and Facebook (EMN.metabolomicssociety) to stay up-to-date on all news and upcoming events.

Task Groups Corner

Precision Medicine and Pharmacometabolomics Task Group

Members of the Precision Medicine and Pharmacometabolomics Task Group led by Dr. Kaddurah-Daouk have been meeting monthly to create awareness on inclusion of metabolomics data in large precision medicine initiatives and in the study of drugs effects.
The group is leading a series of white papers that address scaling up metabolic profiling capabilities, miniaturization, and standardization and harmonization to enable large studies in precision medicine. Other topics of interest to the task group include enabling academic centers to be a part of large studies, issues related to making publicly available large data, lobbying and outreach highlighting the importance of metabolomics, role of exposome diet and gut microbiome in precision medicine and precision health. If you are interested please reach out and join our team (kaddu001@mc.duke.edu).

International Affiliates Corner

11th Scientific Days of the Réseau Francophone de Métabolomique et de Fluxomique (RFMF)

Venue: Théâtre de Liège, Liège, Belgium. May 23-25, 2018

The réseau francophone de métabolomique et de fluxomique (http://www.rfmf.fr) is pleased to invite you to their annual scientific days. This conference will cover the major scientific fields of metabolomics and fluxomics with a special focus on the clinical, health and medicines applications. It will give the opportunity for the scientists coming from the French-speaking communities or not to meet and share in an environment that combines good science and good human relationships. At the scientific level, we are honored to announce the presence of prestigious speakers: Christine des Rosiers (Montréal University), Bénédicte Elena (Institut des Sciences Analytiques from Lyon), Young Hae Choi (Leiden University), Serge Rudaz (Genève University), and Jules Griffin (Cambridge University).

These days will be preceded by a workshop day (May 22, 2018) with sessions dedicated to early-career scientists and PhD students.

Swiss Metabolomics Society (SMS)

Visit: www.swiss-metabolomics.ch

Join us for the next General Assembly on the 14th of November 2018 in Bern. The General Assembly will be combined with a scientific event.
Please visit **www.swiss-metabolomics.ch** to get the latest updates.

SpOtlight

Spotlight Article Contributed by:

Steffen Neumann - Researcher, Department of Stress and Developmental Biology, Institute of Plant Biochemistry, Halle, Germany
Dejan Nikolic - Research Associate Professor, Department of Medicinal Chemistry and Pharmacognosy, College of Pharmacy, University of Illinois at Chicago, US
Emma Schymanski - Head of Environmental Cheminformatics Group, Luxembourg Centre for Systems Biomedicine, University of Luxembourg, Luxembourg
Nir Shahaf - Scientific advisor, Department of Plant and Environmental Sciences, Weizmann Institute of Science, Israel

Critical Assessment of Small Molecule Identification:

Looking at the 5th Edition of CASMI

The Critical Assessment of Small Molecule Identification,or CASMI for short, is a contest on small molecule identification using mass spectral data. The fifth edition finished in October 2017. The contest challenge spectra in Category 1 to 3 were contributed by Dejan Nikolic, and for Categories 2 to 4 by the Aharoni lab at the Weizmann Institute of Science. Figure 1 shows some examples, and the structural diversity of the challenge structures.

Participants were required to submit a ranked list of candidate structures per challenge spectrum.

An identification is considered correct if a submitted structure has the same connectivity as the correct solution, which is checked by the first block of the InChI Key. If the correct solution was ranked first in a candidate list, 25 points were awarded, 18 points for second, down to one point for 10th place, as performed in Formula One Racing. The sum of these F1 scores was used to rank the performance of all participants in a Category. This year the contest consisted of four categories.

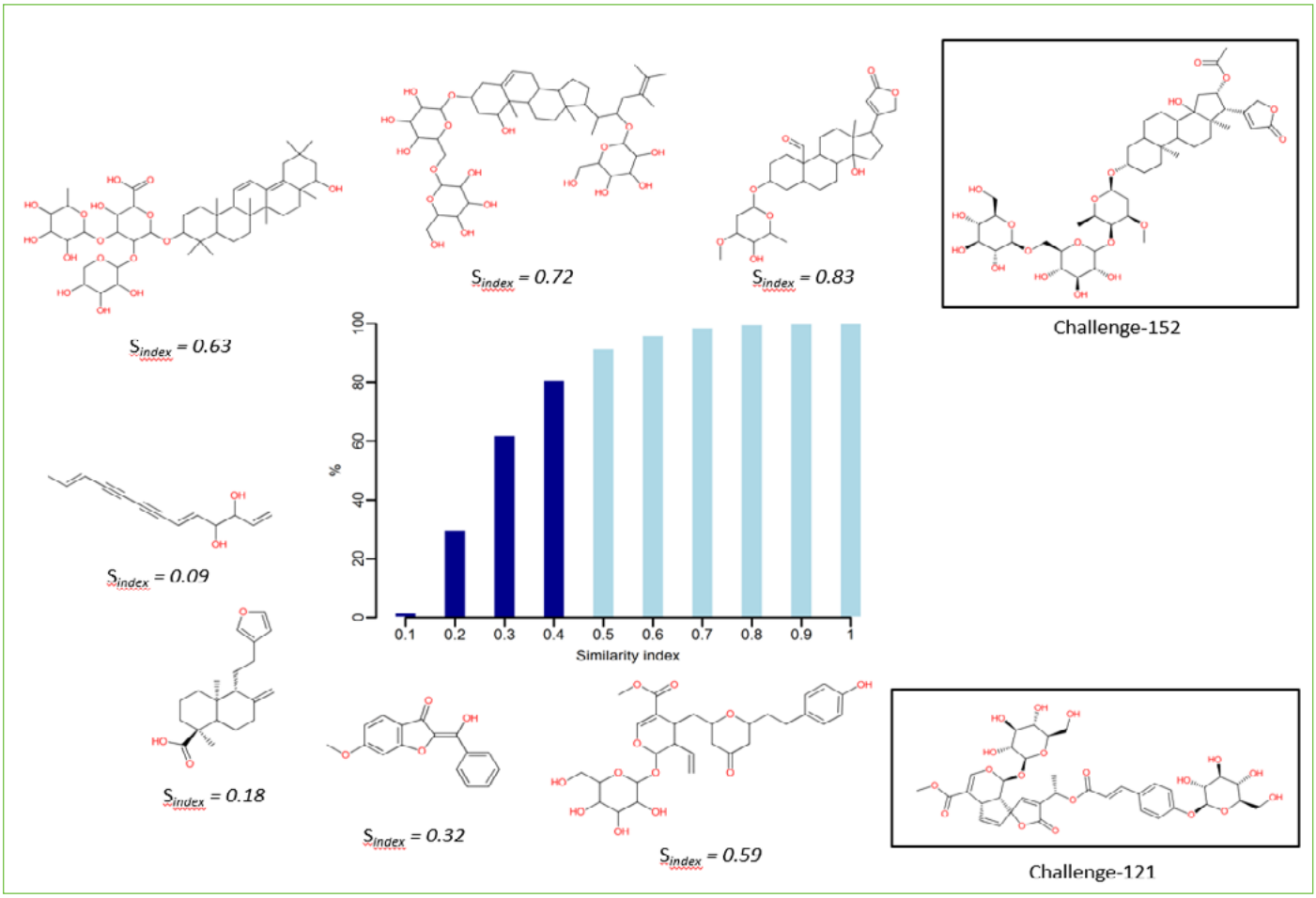


Figure 1: Chemical diversity of the contest structures for challenges 46 to 243, consisting of plant-related metabolites. The cumulative structural pair similarity values are depicted as a bar plot, the pair-values with similarity index values <= 0.4 shown in dark blue, thus indicating a common threshold for structurally unrelated compounds and illustrating the high overall structural diversity of the challenge structures. Structures at top and bottom are examples with increasingly higher similarity indices ("Sindex") relative the example structures (Challenge 121, PubChem CID5862036 and Challenge 152, PubChem CID14585037).

Category 1 was "Best Structure Identification on Natural Products" on Challenges 1-45. All kinds of approaches, including manual, semi-automatic and automatic were allowed and encouraged. The winner, Team Dührkop, had already participated in previous years, and submitted 2017 entries using two variants of the CSI:FingerID software, achieving 24.4% correct solutions ranked first. Catherine Stacey (US) was a new participant in CASMI, achieving 15.6% ranked first. Her scoring was based on molecular formula calculations and fragmentation rules developed with OpenBabel. Samuel Bertrand (Université de Nantes, France) had already participated in earlier CASMI contests. He used a workflow with molecular formula calculation and searching in several structure databases. The scoring used a combination of CFM-ID and the spectrum comparison in Tremolo library search software. Information about the phylogeny of the species and databases was also included and individual scores were then summed up. Another new entry to CASMI was team Botella (SEESLAB, Catalonia, Spain). They used a set of tools, including MS-FINDER, MetFusion, CFM-ID, and their own iMet taking biochemical reactions into account. The individual scores were integrated with a Bayes model to obtain a final score.

	F1 Score	Median Rank	Top	Top3	Top10	Missed Solutions
Team Dührkop	**469**	4	**11**	**19**	**28**	**4**
C. Stacey	330	3	7	13	17	22
S. Bertrand	319	4	6	12	21	16
Team Botella	237	13	4	10	15	12
Team Kumar	192	**1**	6	8	9	36

Table 1: Participant summary for Category 1, the F1 score is a weighted sum of the ranks. All details are available at www.casmi-contest.org. Best results per column are bolded.

The team around Rakesh Kumar (ICGEB, New Delhi, India) was another first-time participant. Their scoring used natural product likeness and metadata information, where available, for respective challenges. They had the best median rank, but missed too many correct solutions to obtain a better overall result.

Three out of five entries in Category **1** were first-time participants, see Table 1 for an excerpt of the results, and the website http://www.casmi-contest.org/2017/ for the complete data.

Categories **2** and **3** involved Challenges 1-243, while Category **4** involved Challenges 46-243.

In Category 2 "Best Automatic Structural Identification - In Silico Fragmentation Only" participants could use any database to retrieve the structures for their candidate lists and in silico methods using the MS/MS fragmentation data only.

In addition to team Dührkop and team Kumar, the team around Yuanyue Li from the Peer Bork group (European Molecular Biology Laboratory, EMBL, Heidelberg, Germany) participated with a machine learning approach to predict the probability spectrum, scoring the similarity between the probability spectrum and real spectrum.

Category 3 "Best Automatic Structural Identification with Full Information, including literature and metadata" only had two participants this year. Here, Tobias Kind (UC Davis, US) had both more top positions and fewer misses than Team Hiroshi Tsugawa (RIKEN, Yokohama, Japan).

In Category 4, in addition to the teams Dührkop, Kumar and Li mentioned above, the team Bach from the group of Juho Rousu (Aalto University, Espoo, Finland) participated with CSI:FingerID and different variants of the updated Input Output Kernel Regression (IOKR), and Team Ruttkies with MetFrag+.

	Category	F1 Score	Median Rank	Top	Top3	Top10	Missed Solutions
Team Dührkop	2	**2775**	**5**	**77**	**110**	**147**	**4**
Team Li	2	942	31	16	31	72	10
Team Kumar	2	109	333	0	0	5	28
Team Kind	3	**3707**	**2**	**91**	**148**	**193**	**34**
Team Tsugawa	3	1559	7	28	56	104	64
Team Dührkop	4	**2306**	**5**	**66**	**91**	**119**	**0**
Team Bach	4	1402	201	36	59	73	**0**
Team Li	4	718	31.5	10	23	58	**0**
Team Ruttkies	4	634	142	6	21	51	**0**
Team Kumar	4	301	135.5	0	2	19	2

Table 2: Summary of performance in Category 2, 3 on 243 challenges, and Category 4 with 198 challenges. Best results per column and category are in bold face. All details are available at www.casmi-contest.org.

Spotlight | *CASMI 2017*

Team Kind led the performance in Category 3, using fragmentation information and their plant metabolite target library. Team Dührkop with CSI:FingerID performed best in Categories 2 and 4, see Table 2 for an overview.

The early CASMI contests also had a category for "best molecular formula" prediction. Some teams solved this already in 2013 by submitting de-duplicated formulas corresponding with the candidate structures.

If this strategy were applied to the 2017 contest in Category 4, Team Li would have led the way with 151 out of 198 molecular formulas ranked first.

Contests like CASMI help to bring together the mass spectrometry community, and determine how well the approaches work on a common challenge set.

A workshop on Metabolite Identification Approaches will also cover CASMI at the 14th International Conference of the Metabolomics Society (Seattle, Washington, USA from June 24-28, 2018).

METABOINTERVIEW

Dr. Horst Joachim Schirra

Honorary Research Fellow
Centre for Advanced Imaging
The University of Queensland (UQ)
Brisbane, Australia

Short Biography

Dr Schirra is one of the leaders of NMR-based metabolomics in Australia. He studied Chemistry at the Johann-Wolfgang-Goethe University (Frankfurt, Germany), and received his PhD in Biochemistry from the ETH Zurich (Switzerland).

In 1999, he joined UQ, where he was awarded a Postdoctoral Fellowship of the Australian Research Council and a prestigious Queensland Smart State Fellowship.

In 2009, Dr Schirra became Lecturer in the School of Chemistry and Molecular Biosciences at UQ, and in 2012 he joined UQ's Centre for Advanced Imaging, where he leads a multidisciplinary research program in Metabolic Systems Biology and manages the Centre's newly established facility for NMR-based metabolomics.

Dr Schirra uses NMR-based metabolomics to investigate the basic principles of metabolic regulation and the role they play in fundamental biological processes, environmental change, and in the development of disease. He aims to integrate metabolomics with other –omics methods and metabolic simulations.

Dr Schirra is a Director of the Metabolomics Society, Board Member of the Australian and New Zealand Society for Magnetic Resonance, and committee member of the Australian and New Zealand Metabolomics Network.

He was co-chair of Metabolomics 2017 in Brisbane. He is editorial board member of the journal *Metabolites*, and regional editor of *Current Metabolomics*.

Interview Q&A

How did you get involved in metabolomics ?

I started my scientific career as an NMR spectroscopist, working on the structural biology and folding of proteins that are of medical interest or important in defending plants against insect pests and other predators [1-6].

In 2004, a colleague from The University of Queensland (UQ) approached me who wanted to study the metabolic consequences of mutations in the growth hormone receptor, which phenotypically lead to late-onset obesity. They had heard about this "newfangled technique" called metabolomics (at that time still "metabonomics"), and were asking whether I could use my NMR skills to do such experiments.

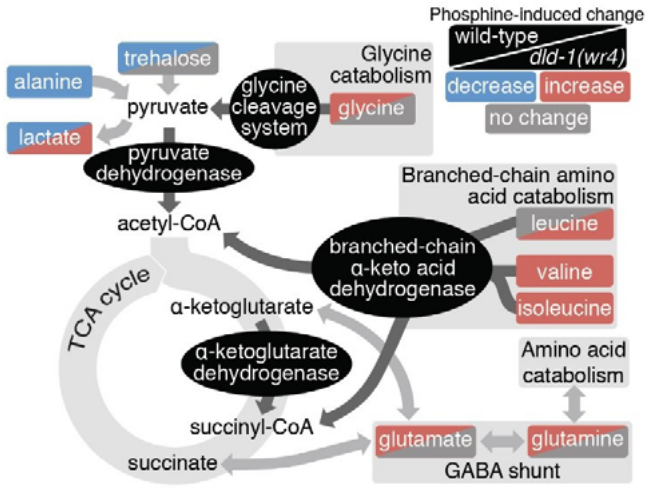
I was excited about trying something new, and in the process we found that taurine is involved in the development of obesity [7]. I realised the potential of metabolomics as a platform technology for investigating the biological ramifications of disease and environmental change, and with word of me doing metabolomics getting out at UQ, I quickly transitioned to systems biology and launched a research program that extended further into clinical metabolomics [8-10], as well as livestock science [11-12], microbial metabolomics [13-14], metabolic regulation and fumigant resistance [15].
The rest, as they say, is history. . .

What are some of the most exciting aspects of your work in metabolomics ?

Grain stores world-wide are safeguarded against pest insects with the fumigant phosphine. Multiple grain storage pest insects have developed a high level of resistance against phosphine in countries across the world, threatening global food security. In a ground-breaking study, together with colleagues from UQ's School of Biological Sciences we have discovered that the core metabolic enzyme dihydrolipoamide dehydrogenase (DLD) is responsible for resistance to phosphine gas in the nematode *C. elegans* as well as every major pest insect of stored grain [15].

We are using that discovery now to characterise the effects of different fumigants that have the potential to overcome phosphine resistance. In addition, it appears that DLD is an underestimated core regulatory enzyme of metabolism [16]. To aid the systems interpretation of this research, we have developed a genome-scale metabolic model (GSM) of *C. elegans* [16-17]. We are now part of the WormJam international research consortium, which joins all metabolomics researchers working on *C. elegans* world-wide, and aims to build a consensus GSM between our model and others that were independently built in parallel [18].

As an interesting footnote on the strange ways science sometimes works: DLD is part of the thiol-disulfide oxidoreductase protein family – the same family to which DsbA belongs, which was subject of my PhD project [1]. That means in an unexpected way I have come full circle, and can now use my expertise in both systems and structural biology to characterise this vital enzyme.



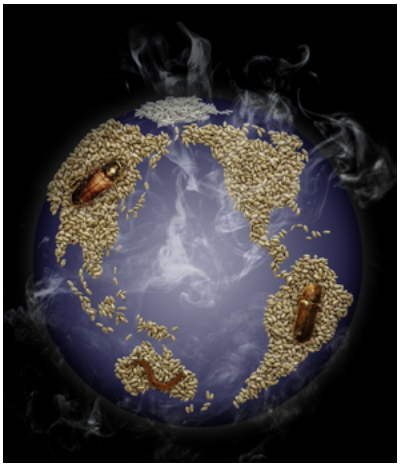


Figure 1:
Left: Phosphine gas is used to protect global grain reserves, which are threatened by the emergence of phosphine resistance in pest insects. (Copyright: Nicholas Valmas, UQ).
Above: The enzyme dihydrolipoamide dehydrogenase (DLD), which is responsible for phosphine resistance in insects and nematodes is involved in several key metabolic pathways (DLD-containing enzyme complexes are shown as black ovals).

Our work on metabolic regulation in livestock has developed into a large program in a long-standing collaboration with Commonwealth Scientific and Industrial Research Organisation (CSIRO) Agriculture partly funded by the industry body Meat and Livestock Australia.

I have conducted one of the first metabolomic studies on ruminants, which uniquely, allowed me to unravel metabolic effects down to the organelle level [11].

This study revealed metabolic downregulation and hypometabolism under limited energy input similar to what I previously observed in *C. elegans*. This hints at common mechanisms of metabolic regulation that are centred on DLD.

Together with colleagues at the UQ Centre for Clinical Research, we work on the development of early and non-invasive diagnosis methods for prostate cancer.

By relating the changes in metabolic profiles of a unique collection of ejaculate and post-ejaculate urine samples from patients to their carefully documented clinical status, we are aiming to overcome the current shortcomings in diagnosis and patient management.

We have studied the reliability of molecular markers in ejaculate [19], developed methods for stabilising the metabolite profile in ejaculate [20], and evaluated the potential for NMR-based metabolomics to stratify patients, based on ejaculate samples [10].

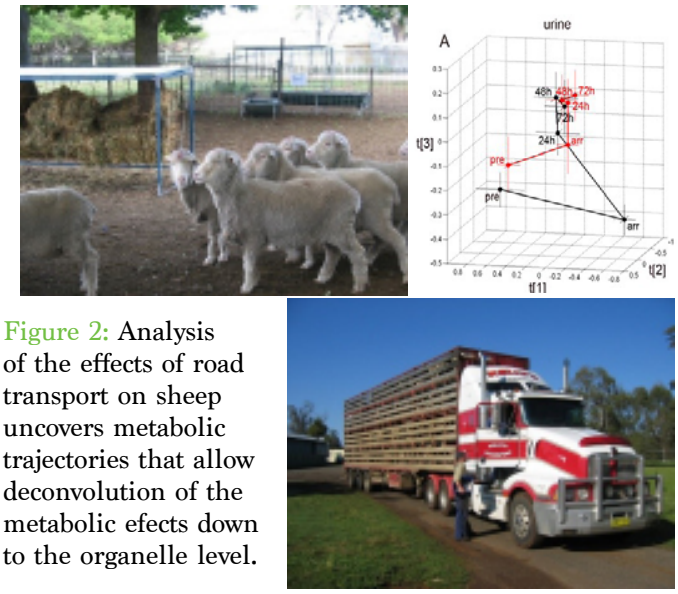


Figure 2: Analysis of the effects of road transport on sheep uncovers metabolic trajectories that allow deconvolution of the metabolic efects down to the organelle level.

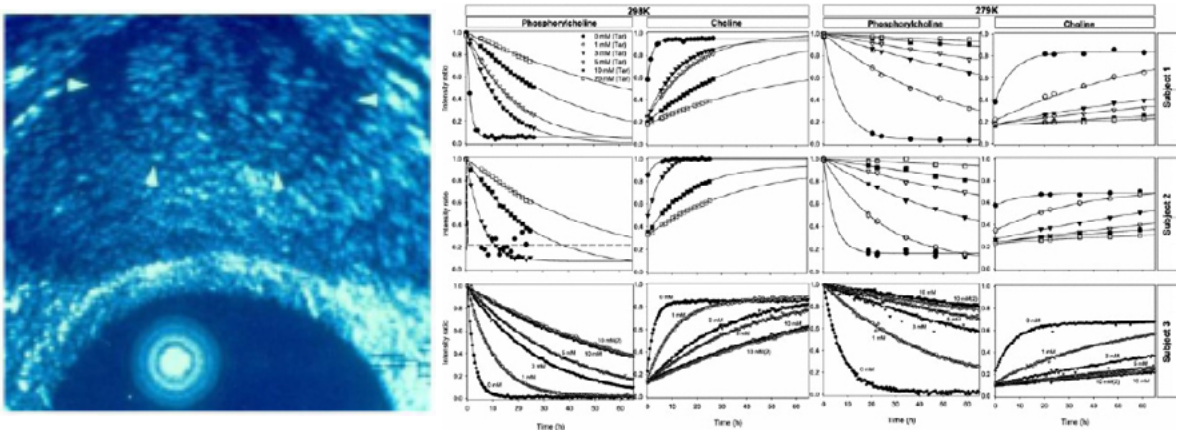


Figure 3: Left: Transrectal ultrasound image of the prostate. **Right:** Taratate inhibits the conversion of phosphocholine to choline in seminal fluid.

MN What key metabolomics initiatives are you pursuing at your research centre or institute ?

The Centre for Advanced Imaging (CAI) runs a large research program in Systems Biology, Metabolomics, and Megavariate Data Analysis, which brings together researchers from within CAI, other UQ faculties and institutes, and research partners nationally and internationally [https://cai.centre.uq.edu.au/research/systems-biology-metabolomics-and-megavariate-data-methods]. CAI has excellent infrastructure for Magnetic Resonance, among them a 900 MHz spectrometer, which is the highest field strength NMR instrument in the Southern hemisphere, a 7T Siemens Magnetom whole-body MRI, and facilities for producing tracers.

Based on the strength of the equipment and the expertise for NMR-based metabolomics, the Centre launched in 2016 the UQ facility for NMR-based metabolomics [https://cai.centre.uq.edu.au/nmr-based-metabolomics]. The facility has instrumentation (the 900 MHz spectrometer, next to a 700 MHz NMR, both equipped with cryoprobes for increased sensitivity and with chilled sample changers for high-throughput sample measurement) and expertise available for all varieties of metabolomics research, and collaborates with researchers and partners within Australia and overseas.

Figure 4: The flagship instruments of the UQ facility for NMR-based metabolomics are a 900 MHz (**left**) and a 700 MHz NMR spectrometer (**middle**). The facility is managed by Horst Joachim Schirra (**right**).

It provides a high-end, integrated metabolomics NMR data acquisition and analysis facility to enhance collaborative biomedical and biological research programs within the University and industry sectors. The facility has grown within its first year of operation, and has achieved a national leadership position in NMR-based metabolomics and systems biology. In addition, the facility is in the process of affiliating with the Queensland node of Metabolomics Australia to increase MA's capacity to offer high-quality reliable services in NMR-based metabolomics.

MN What is happening in your country in terms of metabolomics ?

Australia is generally punching well above its weight when it comes to metabolomics, e.g., after Americans, Australians are the second largest group of members in the Metabolomics Society, well ahead of some larger European countries (maybe we need "The Ashes" (Test cricket series played between England and Australia) in metabolomics as well?).

The biggest recent thing happening in Australia was the Metabolomics 2017 conference in Brisbane. We were able to welcome ~550 scientists from all over the world to our beautiful city, and as co-chair it was a very pleasurable adventure to organise the conference. And we were the first conference of the Metabolomics Society in the Asia-Pacific region to not make a loss – a feat the whole local organising committee (LOC) is quite proud of.

The other big news is happening on the other side of the continent, with the recent establishment of the Australian Metabolic Phenotyping Centre (AMPC) in Perth, which was established in 2017 [http://www.wahtn.org/enabling-platforms/australian-national-phenome-centre/]. The AMPC is the first Phenome Centre in Australia, and is part of the International Phenome Centre Network. Some really nice work is expected to come out of that corner of the country.

Especially, the NMR community has embraced metabolomics over the past years. Several groups, including mine, are doing NMR-based metabolomics, the UQ facility for NMR-based metabolomics has been operational since 2017, and more facilities like it will become available over the next few years.

This demand has led the Australian and New Zealand Society for Magnetic Resonance (ANZMAG) to invite David Wishart as the ANZMAG lecturer in 2016. David toured Australia and NZ, and gave a week-long course on NMR-based metabolomics at UQ, which has been recorded, and is now available for everyone to watch on the ANZMAG YouTube channel [https://www.youtube.com/user/ANZMAG/playlists].

MN How do you see your work in metabolomics being applied today or in the future ?

Our work on DLD has the potential to uncover fundamental mechanisms of metabolic regulation, which are important in all kinds of biological and clinical phenomena from hypometabolism, hibernation, longevity, and fumigant resistance, to inflammation and malignant transformation [16].

The computational consensus model of *C. elegans* metabolism that we are developing will be useful for anyone working on this important model organism [16-18]. Our work on developing alternative pest control strategies using a systems biology approach has led to the discovery of a phosphine synergist with commercial potential and has already had a direct impact on grain growers in Australia.

Metabo Interview | *Dr. Horst Joachim Schirra*

As you see it, what are metabolomics' greatest strengths ?

Metabolomics is by virtue of measuring metabolite levels very close to the phenotype. It is possible to get a systemic picture relatively quickly. Metabolomics integrates well with genome-scale modelling as well as with other –omics/ systems biology approaches. All these features have led to a renaissance of metabolism research in recent years, making it very exciting to work in this field.

What do you see as the greatest barriers for metabolomics ?

Metabolite identification is in my opinion the single biggest bottleneck in the metabolomics pipeline.

There are several initiatives underway to alleviate this situation and elucidate the "dark matter" of the metabolome. One observation is that people in the metabolomics field are at the moment underutilising skills in metabolite identification that are present and routine in both the natural products chemistry and analytical chemistry field.

E.g., the structure identification of novel, and often quite complex, metabolites with NMR spectroscopy is quite routine in the natural products field – and fast. The other observation is that metabolite identification work is at the moment a thankless task. Putting the hard yards in costs time and resources, and will not yield any rewards in term of publication or recognition – and sometimes it turns out the metabolite you identified was described 50 years ago in some obscure organic chemistry journal, and the identification data never made it into publicly accessible modern databases.

Maybe it is time for the metabolomics field to create a publication category of "(re-)identification of metabolite XXX" – similar to the "crystallisation of protein XXX" papers of X-ray crystallography, or the "sequential NMR assignment of protein XXX" of NMR-based structural biology – a small one–page affair, in which credit could be given to high-quality metabolite identification data, and whose content could then quickly flow on into databases.

The other barrier is the biological interpretation: You have just identified your list of significant metabolites that are changing in your system, and now what? Methods of pathway analysis, and network analysis are still in their infancy and only as good as the curation they are based on. Effectively, we are still stuck at the "highlight your metabolites with a yellow texta on the old metabolic pathways chart and see what you get"-stage.

One potential avenue out of this is the advent of genome-scale metabolic models (GSMs) [22]. GSMs assemble all metabolic reactions that an organism is capable of into a computational model that then allows one to simulate metabolism under different conditions, and to calculate metabolic fluxes through individual pathways [22]. GSMs are a natural partner for both metabolomics and other –omics sciences as they allow the integration of different types of –omics data. In this way the integration of your metabolomics data with GSMs would enable estimation of metabolic fluxes – a much more consistent approach than the "texta" method. In addition, they are a promising avenue for conducting multi-omics studies, and the combination of metabolomics with GSMs can lead to an iterative cycle, where GSMs enable the interpretation of metabolomics data, and metabolomics data aid the improvement/refinement of GSMs in turn [22] – a win-win situation for both fields. It is no coincidence, that these two topics were the major feature themes of the 2017 Metabolomics conference in Brisbane.

What improvements, technological or otherwise, need to take place for metabolomics to really take off ?

Metabolomics is thankfully a fast evolving field where researchers are generally aware of the limitations and are actively trying to overcome them. Some of the frontiers and challenges that I see are:

- **Interdisciplinarity:** Metabolomics needs to improve and tighten its communication and scientific exchange with researchers in cognate fields such as genomics, proteomics, systems biology, genome-scale modelling, and natural products chemistry/analytical chemistry

- **Spatially-resolved metabolomics** is coming along by leaps and bounds. But the development of analytical methods for spatial metabolomics data needs to catch up.

- Similarly, **the analysis of time-resolved metabolomics data** is a challenge in that multiple methods have been suggested, but – unlike the standard multivariate approach for time-independent data - a universally accepted workflow/analysis scheme has not yet emerged.

- **Increasing the sensitivity and decreasing the sample size** is a constant push in metabolomics and nowhere is that more visible than in the emerging field of single-cell metabolomics.

- **Cost:** Related to increasing sensitivity it is important for metabolomics to develop its methods, workflows and technologies so that the costs per sample become increasingly lower, making it more affordable for researchers to engage in and with metabolomics research.

- **The deposition of data** has to become routine in metabolomics. We need to routinely deposit the raw experimental data and metadata of any study performed to allow future meta-studies and –analyses. In addition, metabolite identification data need to be routinely deposited – and such deposition should be rewarded - to speed up the bottleneck of metabolite identification.

- **Training** in metabolomics is important for the future of the field. Training of students and researchers new to the field, training of collaborators to establish well-designed metabolomics studies, mutual training of colleagues within the field so that everyone can take advantage of the multiple and rapidly evolving metabolomics techniques and subdisciplines.

How does the future look in terms of funding for metabolomics ?

Generally, the future does not look too bad. Funding agencies, such as NIH and the EU clearly understand the importance of metabolomics and systems biology in both basic research and applied health sciences. In Australia, grant funding has been generally becoming more challenging in recent years thanks to government funding of the major grant agencies being stagnant or even decreasing in real terms. In 2015, R&D funding from Australia's government sat at 0.4% of GDP [23], which puts it second last among OECD countries, behind Greece and just ahead of Slovakia and Spain – clearly there is room for improvement. Metabolomics is occasionally still seen as a "young/immature" technology, especially in the medical research space, where the idea of characterising problems on a systems level is still often seen as a "fishing expedition" by assessors that were trained to think in single specific biomarkers.

What role can metabolomics standards play ?

Standards are critical! Often enough, papers don't have method descriptions that allow reproduction of the experiment. The availability of minimum reporting standards, and the push for deposition of experimental data in databases are crucial to overcoming this barrier. The development of SOPs for conducting metabolomics work and of minimum quality/reporting standards will further increase the quality of the field. In addition, the availability of standard materials and reference substances (e.g., NIST) are also critical to establish long-term reliability in metabolomics studies.

Do you have any other comments that you wish to share about metabolomics ?

After all those years I am still excited to work in this fascinating research area and to see where it will take me – and I am equally happy to share this passion with my colleagues and students. If you too are intrigued: get involved, and let's talk!

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Recent Publications

Recently published papers in metabolomics

- Challenges and emergent solutions for LC-MS/MS based untargeted metabolomics in diseases.
- SWATHtoMRM: Development of High-Coverage Targeted Metabolomics Method Using SWATH Technology for Biomarker Discovery.
- Chemometrics comparison of GC-MS and comprehensive two-dimensional gas chromatography with time-of-flight mass spectrometry Daphnia magna metabolic profiles exposed to salinity.
- An UHPLC-TOF MS metabolomic approach to study the impact of moderate red wine consumption on urinary metabolome.
- Metabolic changes associated with papillary thyroid carcinoma: A nuclear magnetic resonance-based metabolomics study.
- Guidelines for Biomarker of Food Intake Reviews (BFIRev): how to conduct an extensive literature search for biomarker of food intake discovery.
- Elastic net regularized regression for time-series analysis of plasma metabolome stability under sub-optimal freezing condition.
- Comparative and integrative metabolomics reveal that S-nitrosation inhibits physiologically relevant metabolic enzymes.
- The evolution of methods for urinary steroid metabolomics in clinical investigations particularly in childhood.
- Identification of seven novel loci associated with amino acid levels using single variant and gene-based tests in 8,545 Finnish men from the METSIM study.

Metabolomics Events

Recent & Upcoming Events

19-21 Mar 2018

4th Annual Metabolomics Symposium on Clinical and Pharmaceutical Solutions through Analysis (CPSA Metabolomics 2018)

Venue:
The University of Florida Clinical & Translational Science Institute, Gainesville, Florida, USA

Plenary Lecture at CPSA Metabolomics 2018!
We are extremely excited and honored to feature Alla Kloss of Sanofi as the Plenary Lecturer for the 4th Annual Metabolomics Symposium on Clinical and Pharmaceutical Solutions through Analysis (CPSA Metabolomics 2018). Her lecture "Applied Metabolomics: The Way to Reduce Element of Surprise in Pharmaceutical Industry" will be a perfect way to begin the symposia and roundtable discussions. Visit the updated program agenda and make plans to join the conversation!

Travel & Accommodation
Prepare now for your Travel & Accommodations for CPSA Metabolomics 2018. Make your hotel reservations at the Hilton University of Florida Conference Center. Reserve your room on-line or call the hotel directly (352-371-3600).

Registration
Registration is open! Click on the CPSA Metabolomics 2018 registration link and register today!

For further information, please visit http://www.cpsa-metabolomics.com/2018/index.shtml

Metabolomics Events

Imperial College London

19-23 Mar 2018

Hands-on LC-MS for Metabolic Profiling

Venue:
Imperial International Phenome Training Centre, Imperial College London, UK

Earlybird: £1750
Standard: £1950

This week long course covers how to perform a metabolic profiling experiment from start to finish. It will cover study design, sample preparation, the use of mass spectrometry for global profiling, targeted methodologies and data analysis.

Day 1: Introductory lectures in mass spectrometry and chromatography, study design and sample preparation, followed by preparation of biological samples for analysis on subsequent days.

Days 2 and 3: Analysis of biofluids through global profiling and targeted analyses; an introductory session to liquid chromatography, followed by sessions on each of the newest QToF and TQ instrumentation. Instrument set up, method development and acquisition will be covered. We have set a maximum of 3 attendees per instrument allowing for hands-on participation by all. Day 3 finishes with introduction to data analysis.

Day 4: Data analysis workshops where attendees will process the data acquired from the previous days, mixed with further statistics lectures, allowing for development of interpretation skills.

Day 5: Application lectures, tips, tricks and troubleshooting, optional trip to the MRC-NIHR National Phenome Centre.

For further information, please visit http://www.imperial.ac.uk/imperial-international-phenome-training-centre/courses/hands-on-lc-ms-for-metabolic-profiling/.

BIRMINGHAM METABOLOMICS TRAINING CENTRE

21-23 Mar & 19-21 Sept 2018

Introduction to Metabolomics for the Microbiologist

Venue:
Birmingham Metabolomics Training Centre, School of Biosciences
University of Birmingham, Birmingham, UK

Limited bursaries are now available for PhD students funded by NERC, which make the registration for this course **FREE** to these students.

This three-day course will introduce the attendees in how untargeted metabolomics can be applied to study microbial systems in academic and industrial research. The course will provide an overview of the metabolomics pipeline from experimental design to sample preparation and data acquisition to data analysis/interpretation.

The course will be led by experts in the field of metabolomics and will include lectures, hands-on laboratory sessions in sample preparation and data acquisition and computer workshops focused on data processing and data analysis.

Topics covered:

- Introduction to metabolomics, both targeted and untargeted approaches
- Experimental design and the importance of quality control samples in untargeted metabolomics
- Analytical strategies applied in metabolomics with a focus on mass spectrometry
- Hands-on laboratory sessions focused on sample preparation and to include metabolic quenching and extraction procedures, intracellular and exometabolome samples and polar and non-polar extraction methods
- Hands-on laboratory sessions focused on sample analysis for untargeted metabolomics studies using an Acquity UPLC coupled to a Xevo QToF mass spectrometer
- Hands-on workshop focused on data processing and data analysis
- Hands-on workshop focused on an introduction to metabolite identification
- Question and answer session with the experts

Level:

The course is aimed at individuals with minimal experience of applying metabolomics in their research and no or limited experience of using a liquid chromatography – mass spectrometer. The attendees will leave the course understanding and being able to apply the metabolomics pipeline in their research.

For more information and to register, please visit https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/introduction-metabolomics-microbiologist.aspx

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BIRMINGHAM METABOLOMICS TRAINING CENTRE

2-27 Mar & 8 Oct - 2 Nov 2018

Metabolomics Data Processing and Data Analysis

Venue: Online

This online course will explore the tools and approaches that are used to process and analyse metabolomics data, we will investigate the challenges that are typically encountered in the analysis of metabolomics data and provide solutions to overcome these problems. The course will be delivered using a combination of short videos, articles, discussions, and online workshops with step-by-step instructions and test data sets. We will provide quizzes, polls and peer review exercises each week, so that you can review your learning throughout the course.

Course Syllabus:

- An introduction to metabolomics
- An overview of the untargeted metabolomics workflow
- The influence of experimental design and data acquisition on data analysis and data quality
- Processing of NMR data

- Processing direct infusion mass spectrometry data
- Processing liquid chromatography-mass spectrometry data
- Reporting standards and data repositories
- Data analysis, detecting outliers and drift, and pre-treatment methods
- Univariate data analysis
- Multivariate data analysis (including unsupervised and supervised approaches)
- The importance of statistical validation of results
- Computational approaches for metabolite identification and translation of results into biological knowledge
- What are the future challenges for data processing and analysis in metabolomics

Level:
The course would be ideally suited to MSc/PhD students or scientists who are in the early stages of analysing metabolomics data. No previous knowledge of the data processing and statistical analysis approaches is assumed, but a basic understanding of the metabolome, and the analytical techniques applied in the metabolomics field would be beneficial. A pre-course recommended reading list will be provided.

For further information and to register, please visit https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/Metabolomics-Data-Processing-and-Data-Analysis.aspx.

BIRMINGHAM METABOLOMICS TRAINING CENTRE

16-17 Apr & 22-23 Nov 2018

Metabolite identification with the Q Exactive and LTQ Orbitrap

Venue:
Birmingham Metabolomics Training Centre, School of Biosciences, University of Birmingham, Birmingham, UK

Limited bursaries are now available for PhD students funded by NERC, which make the registration for this course **FREE** to these students.

This 2-day course will provide a hands-on approach to teach the latest techniques and tools available to perform metabolite identification. We will apply these tools on the Q Exactive and LTQ Orbitrap mass spectrometry family. The course is targeted towards students and researchers who are actively applying metabolomics.

The course will be led by experts in the field and include significant hands-on experience using both the Q Exactive and LTQ Orbitrap instruments to perform:

- Data dependent acquisition
- Data independent acquisition
- MS/MS and MSn data acquisition

The course will finish with a session on the tips and tricks from the experts and an opportunity to ask questions.

For further information and registration details, please visit http://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/metabolite-identification.aspx or contact bmtc@contacts.bham.ac.uk.

Metabolomics Events

Skaggs School of Pharmacy and Pharmaceutical Sciences
UNIVERSITY OF COLORADO ANSCHUTZ MEDICAL CAMPUS

17-20 April 2018

Hands-On Metabolomics Workshop

Venue:
Skaggs School of Pharmacy, University of Colorado Anschutz Medical Campus, Aurora, Colorado, USA

The Reisdorph Lab is offering Hands-On Workshops at the Skaggs School of Pharmacy on the University of Colorado Anschutz Medical Campus in Aurora, CO. Participants will learn introductory metabolomics or proteomics science and applicable protocols and technologies through a comprehensive, hands-on exploration of typical mass spectrometry-based workflows. Class size is limited to 10 participants to ensure excellent participant-to-instructor ratios. Workshops include topics such as experimental design, sample preparation, mass spectrometry basics, data acquisition, advanced technologies, and quantitative analyses. Over one-half of the workshop is spent in the laboratory performing sample preparation or acquiring/analyzing data on mass spectrometers. Several lectures and laboratories focus on data analysis strategies.

These workshops are appropriate for individuals with little to no experience in mass spectrometry and/or high-performance liquid chromatography (HPLC), who desire a comprehensive overview of metabolomics or proteomics, including bioinformatics. Individuals who are considering incorporating metabolomics or proteomics into their own research would also greatly benefit from these workshops, and include:

- Principal investigators
- Medical Researchers
- Graduate Students and Post-Doctoral Fellows
- Mass Spectrometry Core Users
- Industry Sales Representatives
- Bioinformaticists
- Others who need to be familiar with typical metabolomics and proteomics workflows

For further information, please visit http://www.ucdenver.edu/academics/colleges/pharmacy/AboutUs/NewsEvents/MetabolomicsWorkshop/Pages/default.aspx.

Metabolomics Events

7 May & 22 Oct 2018

Introduction to Metabolomics for the Clinical Scientist

Venue:
Birmingham Metabolomics Training Centre, School of Biosciences
University of Birmingham, Birmingham, UK

This 1-day course in partnership with the Phenome Centre Birmingham will provide clinicians with an overview of the metabolomics pipeline, highlighting the benefits of the technique to the medical field. The course will provide an:

- Introduction to experimental design and sample collection
- An overview of both the analytical and computational methods applied in the field
- Case studies and panel discussions with the experts

For further information and registrations details, please visit http://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/introduction-metabolomics.aspx or contact bmtc@contacts.bham.ac.uk

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15-17 May & 19-21 Nov 2018

Metabolomics with the Q Exactive

Venue:
Birmingham Metabolomics Training Centre, School of Biosciences
University of Birmingham, Birmingham, UK

This 3-day course will introduce you to using the Q Exactive mass spectrometer in your metabolomics investigations. The course is aimed at students and researchers with minimal previous experience of applying LC-MS in metabolomics. The course will be led by experts in the field and include lectures, laboratory sessions and computer workshops to provide:

- An introduction to metabolomics and using the Q Exactive mass spectrometer in your studies
- Polar and non-polar sample preparation for profiling and targeted studies
- Data acquisition for profiling and targeted studies
- Data processing and data analysis
- Introduction to metabolite identification

The course will finish with a question and answer session with a panel of experts.

For further information and registrations details, please visit http://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/introduction-metabolomics.aspx or contact bmtc@contacts.bham.ac.uk

Metabolomics Events

16-17 May 2018

2nd Annual Ohio Mass Spectrometry and Metabolomics Symposium

Venue:
Blackwell Inn, Ohio State University, Columbus, Ohio, USA

The 2nd Annual Ohio Mass Spectrometry and Metabolomics Symposium will be held at the Blackwell Inn at The Ohio State University in Columbus, Ohio, on May 16-17, 2018.

This joint meeting of the 2nd Annual Conference on Food and Nutritional Metabolomics for Health and the 15th Annual Ohio Mass Spectrometry Symposium will build on the success of the inaugural May 2017 joint meeting, which was attended by 234 individuals representing 42 academic and industry organizations. The purpose of this two-day event is to provide an opportunity for academic and industrial researchers to present their findings, share information, discuss research challenges with colleagues, and spark new collaborations.

Registration will open in February. Please visit go.osu.edu/omsms2018 for up-to-date information about the symposium and links to registration.

7-8 June 2018

Quality Assurance and Quality Control in Metabolomics

Venue:
Birmingham Metabolomics Training Centre, School of Biosciences
University of Birmingham, Birmingham, UK

Limited bursaries are now available for PhD students funded by NERC, which make the registration for this course FREE to these students.

This two-day course will provide a comprehensive overview of the application of quality assurance (QA) and quality control (QC) in metabolic phenotyping. The course is aimed at students and researchers who are actively working in the field. Experts who have developed the application of QA and QC procedures within the field will lead the course. It will include both theoretical and practical components to:

- Introduce QA and QC in metabolic phenotyping
- The application of QA and QC in untargeted and targeted studies
- Preparation of QCs and data acquisition
- Data processing and reporting standards

The course will finish with a question and answer session with a panel of experts.

For further information and registration details, please visit http://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/quality-phenotyping.aspx or contact bmtc@contacts.bham.ac.uk

Metabolomics Events

UCDAVIS GENOME CENTER

11-13 June 2018

Workshop: "I Ran My Metabolomics - Now What?"

Venue:
Genome Center of the University of California, Davis, California, USA

A three-day workshop on cheminformatics applications to metabolism research comprising formal lectures and hands-on instruction will be held at the Genome Center of the University of California, Davis from the 11th to the 13th of June, 2018.

This workshop is free of charge and it will include the use of the MINE Database and tools as well as other cheminformatics and bioinformatics programs instrumental to biochemists, physiologists, and biologists working in metabolism.

Our workshop is also suitable for researchers in the fields of medicine and synthetic biology who need an update in state of the art metabolomics.

Metabolomics Association of North America (MANA) travel grants for graduate students and postdocs

Find here all the paperwork:

- General Registration
- Criteria to grant faculty members $1000 travel support
- Travel Support Application Form for Faculty
- Criteria to grant students travel support
- Travel Support Application Form for Students

For further information, please visit http://fiehnlab.ucdavis.edu/events/special-events.

Metabolomics Events

25-28 June 2018

Metabolomics 2018

Venue:
Washington State Convention Center, Seattle, Washington, USA

We are delighted to invite you to the **14th International Conference of the Metabolomics Society**, which will be held in Seattle, Washington, USA, June 24-28, 2018, at the Washington State Convention Center in downtown Seattle. The Convention Center boasts award winning catering, nearby accommodations and dining options within easy walking distance, direct air connections to major cities worldwide and excellent local transportation. Seattle, in addition to being situated in the beautiful Pacific Northwest, is a major hub for science and technology, and is home to more than 25 research institutions and many major companies with global reach.

The conference has an overall goal of **Making Connections**, with major scientific themes of systems biology, big data, technology advances, precision medicine and translational science, plant metabolomics, the microbiome, and the exposome, including environmental and nutritional metabolomics. In addition, the conference will provide many networking opportunities to help establish connections for early career scientists and metabolomics scientists across the Pacific Rim as well as globally.

For further information, please visit http://metabolomics2018.org/.

Metabolomics Events

23-25 July 2018

Multiple biofluid and tissue types:
From sample preparation to analysis strategies for metabolomics

Venue:
Birmingham Metabolomics Training Centre, School of Biosciences, University of Birmingham, Birmingham, UK

Limited bursaries are now available for PhD students funded by NERC, which make the registration for this course FREE to these students.

This 3-day course will provide a comprehensive overview of dealing with complex biological samples for LC-MS analysis. The course is targeted towards students and researchers who are actively applying metabolomics in their research. The course will be led by experts in the field and include:

- An overview of quenching and extraction strategies for different biological samples
- Hands-on sample preparation using different sample types
- Hands-on HILIC and reversed phase LC-MS data acquisition
- Solid phase extraction clean up methods
- An overview of data analysis and metabolite identification
- An opportunity to ask questions and seek advice to prepare samples in your own research

For further information and registrations details, please visit http://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/introduction-metabolomics.aspx or contact bmtc@contacts.bham.ac.uk

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6-9 Aug 2018

1st Annual North American Mass Spectrometry Summer School

Venue:
University of Wisconsin-Madison, Madison, Wisconsin, USA

Organizers:
Josh Coon, Mike Sussman, Lingjun Li, and Dave Pagliarini

Thank you for your interest in the 1st Annual North American Mass Spectrometry Summer School held on the University of Wisconsin-Madison campus.

While we anticipate many of our participants to be graduate students or postdocs, we encourage anyone interested in learning more about mass spectrometry to apply.

Please keep in mind as you continue, that the following application only shows your interest in participating in the Summer School. Once completed, the Organizers will consider all applications and accept students on a rolling basis.

Metabolomics Events

The NSF- and NIGMS- funded North American Mass Spectrometry Summer School (August 6-9, 2018 at University of Wisconsin, Madison) invites applications for travel grants. **A maximum of 50 scholars will receive accommodation, and 10 scholars will receive funds to cover airfare.** Decisions will be based on scientific justification to receive training, scholarly excellence (for different levels of experience), funding need and alignment with NSF- and NIH- criteria (encouraging applications from scientists from underrepresented minorities). **Applications end by April 1st, 2018** but decisions are made on a rolling basis - apply early!

Conference Flyer

For more information about the Summer School, visit https://uwmadison.eventsair.com/massspectrometry/reg/Site/Register

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30 Aug - 1 September 2018

The Australian & New Zealand Metabolomics Conference

Venue:
University of Auckland, New Zealand

The essence of any conference lies in community-building. A meaningful conference is a safe, supportive and open environment aimed at fostering growth, awareness and learning – and should be attendee-driven. These key ingredients for 'reengineering the traditional conference' are the basis and inspiration behind developing ANZMET as the **first peer-driven scientific conference in Australia.** The conference hosts a blend of traditional presentations, roundtable discussions and peer sessions, providing a flat hierarchy and a rich & rewarding interpersonal process.

Following on from the success of the first ANZMET conference in 2016, and its satellite event/workshop held during the Metabolomics2017 conference in Brisbane, Australia, it is with great pleasure and excitement that we continue to develop the peer-conference model and reach out to the dynamic and supportive people of the Australian & NZ metabolomics community.

The ANZMET conference (www.anzmet.org) is designed from conception as a community-owned event and provides a facilitated networking experience where:

(1) Attendees learn on the first day of each others interests, experience, scientific background, collaboration opportunities and other avenues for outreach
(The Round-table Discussion)

(2) An open-forum format for rich discourse on spontaneous peer-selected topics
(The Peer Session)

(3) The delivery of critical updates in the field **(Traditional Presentations)**

(4) The tailored and vital exposure of young scientists to the wider research community
(Rapid-fire Postgraduate Presentation Sessions)

Registrations are **NOW OPEN**! Please visit http://www.anzmet.org/.

Metabolomics Events

BIRMINGHAM METABOLOMICS TRAINING CENTRE

27-28 Sep 2018

Introduction to Metabolomics for the Environmental Scientist

Venue:
Birmingham Metabolomics Training Centre, School of Biosciences, University of Birmingham, Birmingham, UK

Bursaries for NERC funded scientists: While this course is open to all researchers with an interest in the environmental sciences, it is a NERC-funded Advanced Training Short Course and hence priority will be given to NERC funded scientists; this includes NERC PhD students (highest priority), NERC PDRA's and Fellows (next highest priority) and principal and co-investigators who currently hold NERC funding.

This 2-day NERC-funded Advanced Training Short Course will provide environmental scientists with an overview of the metabolomics pipeline. The course is intended for environmental scientist with little or no previous experience of metabolomics and who are interested to discover how this relatively new and powerful approach could be integrated into their research. Experts working in the NERC Metabolomics facility-NBAF-Birmingham will teach the course.

Topics covered:

- Introduction to environmental metabolomics with case studies
  Experimental design and quality control
- Sample collection and preparation
- Overview of analytical laboratory techniques
  (mass spectrometry and NMR spectroscopy)
- Overview of data processing and statistics for metabolomics
- Introduction to metabolite identification

For further information and registration details, please visit https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/introduction-metabolomics-environmental.aspx or contact bmtc@contacts.bham.ac.uk

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If you know of any metabolomics lectures, meetings, workshops, or training sessions that we should feature in future issues of this newsletter, please email Ian Forsythe (metabolomics.innovation@gmail.com).

Metabolomics Jobs & Collaborations

If you have a job you would like posted, please email Ian Forsythe (metabolomics.innovation@gmail.com). Job postings will be carried for a maximum of four issues (eight weeks) unless the position is filled prior to that date.

Jobs Offered

Job Title	Employer	Location	Posted	Closes	Source
Postdoctoral Researcher Position	UCSF	San Francisco, USA	01-Mar-18	Until filled	Metabolomics Society Jobs
Postdoctoral Position (Bioinformatics / Metabolomics)	Brigham and Women's Hospital / Harvard Medical School	Boston, USA	27-Feb-18	01-Jun-18	Metabolomics Society Jobs
Senior Scientific Officer (Lipidomics/ Metabolomics)	Nanyang Technological University	Singapore	12-Feb-18	Until filled	Metabolomics Society Jobs
Postdoc Position in Cheminformatics and Computational Metabolomics	Friedrich-Schiller-University	Jena, Germany	09-Feb-18		Friedrich-Schiller-University
Tenure Track Faculty Position in Food and Nutritional Metabolomics	The Ohio State University	Columbus, USA	02-Feb-18	02-Aug-18	Metabolomics Society Jobs
Ph.D. Position on Mass Spectrometry-Based Analysis of Metabolites	University of Basel	Basel, Switzerland	31-Jan-18	Until filled	Metabolomics Society Jobs
Various Positions			29-Jan-18		Metabolomics Association of North America
Postdoctoral Fellow in Metabolomics and Exposomics	Icahn School of Medicine at Mount Sinai	New York, USA	26-Jan-18	Until filled	Metabolomics Society Jobs
Senior Research Assistant in Metabolomics	Icahn School of Medicine at Mount Sinai	New York, USA	24-Jan-18	Until filled	Metabolomics Society Jobs

Metabolomics Jobs |

Jobs Wanted

This section is intended for very highly qualified individuals (e.g., lab managers, professors, directors, executives with extensive experience) who are seeking employment in metabolomics.

We encourage these individuals to submit their position requests to Ian Forsythe (metabolomics.innovation@gmail.com). Upon review, a limited number of job submissions will be selected for publication in the Jobs Wanted section.

- ***There are currently no listings***