MetaboNews

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In This Issue

Ian Forsythe
Editor
Department of Computing Science
University of Alberta, Canada
metabolomics_innovation@gmail.com

Devin Benheim
Contributing Editor
Department of P,A&M
La Trobe University, Australia
devin.benheim@anzmet.org

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

Welcome to the May 2018 issue of MetaboNews! We have been humbled by the overwhelming response to our new and exciting format from the metabolomics community and our loyal subscribers. As we continue our journey into the new format, do please remember to reach out to the editors with suggestions, ideas and content at any time.

Metabolomics Society News

Metabolomics 2018 Updates

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 will feature the latest and greatest advances across the full range of metabolomics science. Make sure to join us as we meet in Seattle, a world-class metropolis set within the beautiful, natural surroundings of the Pacific Northwest. Registration is still open at http://metabolomics2018.org/.

Workshops are still available for signup as part of the Registration process. This year we will hold 15 workshops, including a Novice Track of 5 workshops and a broad range of more advanced workshops. Space is limited so sign up quickly.

A number of networking and other events have also been announced, including a Forum on Metabolomics Research Cores, a Town Hall Forum for the Society, and events for the Early Members Network, Pacific Rim scientists and the Metabolomics Association of North America. And don't miss out on the exciting conference dinner to be held at the Museum of Popular Culture (MOPOP). See you in June in Seattle!

Metabolomics 2019

Metabolomics 2019 will be organized in the World Forum in The Hague, The Netherlands. It is the Hague's largest convention centre and very close to the seaside. "The Netherlands Metabolomics Centre (NMC) is proud that the Hague has been chosen as the European destination for the 15th Annual Conference of the Metabolomics Society. The conference will take place over five days on June 24-28, 2019," explains Merlijn van Rijswijk, director of NMC.

"In the conference we will put a strong emphasis on the applications of metabolomics and collaborate with other national societies in Europe and beyond, to make as many travel grants available for young researchers as possible. We will be reaching out to other communities, for instance the Biobanking community in Europe, that are increasingly applying metabolomics in their research, but not doing the analyses themselves. Therefore, we expect to attract a record number of attendees from all over the world," says Thomas Hankemeier, Scientific Director of NMC and Chair of the Local Organizing Committee.

Jules Griffin
Metabolomics Society President

Board of Directors

Words From the President

This month one of our tasks was to approve the affiliation of the Metabolomics Association of North America, or MANA, I am very happy to report that the Board unanimously endorsed this affiliation and MANA join a number of local affiliation networks that circle the globe. As part of this affiliation process we (the Society and affiliates) agree to work together to promote metabolomics for the whole community, and on a more practical level often assist one another in putting on conferences and workshops.

We currently have a number of regional organisations interested in affiliating including a new network in South Africa and Metabomeeting in Europe. However, there are parts of the globe where we are struggling to make contact with regional organisations, in particular much of Africa and South America. So if you are reading this in that part of the world I would encourage you to make contact with the Society and we can work together to develop the field both locally and internationally.

Affiliates can apply for financial assistance in putting on local meetings and we might even stretch to flying in a big name to promote the field - although probably wait for next financial year for that one!

Members Corner

Early Career Network (EMN)

EMN Webinar Series – 2018
An EMN webinar was held on April 24th 2018. Dr. Oliver Fiehn (Director of the NIH West Coast Metabolomics Center at UC Davis) presented "Use better software: MS-DIAL instead of XCMS, ChemRich/MetDA instead of Metaboanalyst". Stay tuned for upcoming webinars.
You can access the recorded videos of the past webinars on the Metabolomics Society website.

EMN Travel Bursary 2018: Winners Announcement!
The Early-career Members Network (EMN) Committee of the Metabolomics Society is pleased to announce the Travel Bursary recipients for 2018. The four award winners are as follows:

For the Student Category

- **Yannick Audet-Delage** from Laval University, Canada
- **Fatema Bhinderwala** from the University of Nebraska-Lincoln, USA

The Metabolomics Society is an indepenent non-profit organisation dedicated to promoting the growth, use and understanding of metabolomics in the life sciences.

General Enquires
info@metabolomicssociety.org
Membership Enquiries
membership@metabolomicssociety.org

For the Postdoctoral Category

- **Katie Hillyer** from Victoria University of Wellington, New Zealand
- **Mary Christine Playdon** from the National Cancer Institute, USA

We thank all applicants with such high-quality applications. Please join us in congratulating the winners who will be awarded $500.00 to attend conferences in 2018 where they will present on their metabolomics-related research.

EMN Workshops at the 14th Annual International Conference of the Metabolomics Society

The EMN will host four workshop sessions (Experimental Design, Intro to Mass Spec Analysis, Statistical Analysis, and a Career Workshop) tailored for the needs of early-career scientists who are new in metabolomics fields. If you plan on attending the conference, please join us!

For more details, please check on the website:
http://metabolomics2018.org/program/workshops

International Affiliates Corner

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

IROA TECHNOLOGIES
...making metabolic profiling easy®

3 Challenges in Metabolomics Analysis ...and a Solution

Challenge 1:

Reproducible Measurements Across Time and Instruments

Metabolomic techniques can identify and crudely quantify several hundreds of compounds in a biological sample. However, unless the samples are analyzed in a single batch relative to a known standard, reproducibility cannot be assured because accumulated variances (from instrument and chromatographic drift, sample preparation etc.) can alter results sufficiently. Further, it is not trivial to achieve reproducible measurements when directly comparing data generated on the same instrumentation several days apart, or even more problematic, different instruments based on the same or different methods[1].

Challenge 2:

Reliable QC Standards and Scoring Method to Validate Metabolomic Data

Quality control standards are essential to measure matrix effects and validate metabolomic data. Plasma and serum are widely used matrices and there has been a concerted effort to develop QC standards that represent these matrices[2].

Pooled aliquots of every sample to be analyzed can be collected so as not to miss any compounds unique to the treatment as compared to control[3,4]; however without sufficient material this is not practical for long-term projects[5]. A huge issue is discerning real compounds from artefacts or determining which of the multitude of peaks to use as standards.

If large pooled samples are obtained, safe handling precautions are necessary, and samples must be carefully monitored as storage conditions and sample preparation may create artefacts and further potential sources of variability that obscure metabolite identification[6]. Furthermore, plasma is unsuitable for cross-platform analysis because the number of differences encountered when using different sources, chromatographic systems, or even detectors will preclude any point of comparison[7].

Along with reliable QC standards, it is essential to have appropriate bioinformatic tools to efficiently process huge datasets and scoring algorithms that compare metabolic information, i.e., orthogonal physiochemical characteristics, against biochemical databases to validate data.

Challenge 3: *A Solution*

Accurate Identification of Compounds

The identification of compounds across different mass spectral techniques is unlikely to be successful without careful calibrations and authentic standards. Multiple biological compounds may be confused because they have the same exact mass. Even more problematic are unknown artefactual or fragmentary compounds that are structurally and chemically different from their biological isobaric equivalents but may share the same mass or formulae, and which typically outnumber known metabolites in metabolomics studies.

MS-based metabolomics methods use isotopically labeled standards to ensure accurate identification as they behave physically and chemically (including ionization efficiency) identical to analytes under measurement[8]. However, for untargeted or complex targeted analyses, it becomes impractical (and unaffordable) to match internal standards to large numbers of unlabeled compounds and their fragments, or to achieve the clean baseline separations that would be needed to do so.

To solve these 3 challenges, we constructed an IROA[9] **Fully Labeled Standard** called **Matrix**. Matrix contains 100s of metabolites labeled at both 5% and 95% U-^{13}C, mixed 1:1, providing **triply redundant QC**. **Figure 1** shows an example of a molecule represented in the Matrix.

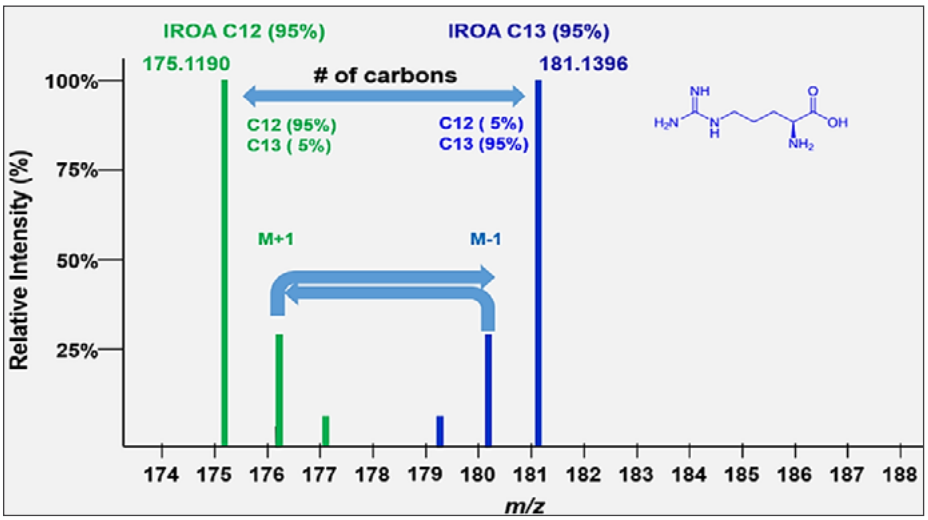

Figure 1: Representation of the IROA-Matrix molecule arginine; IROA labeled with 5% and 95% U- ^{13}C and mixed 1:1 which gives rise to an isotopomeric collection of peaks: both the 95% envelope (95% U-^{13}C peaks; M-1, M-2 etc.) and its mirror-image 5% envelope (5% U-^{13}C peaks; M+1, M+2 etc.). Every molecule in the Standard presents itself as a collection of peaks with the mass distance between each peak exactly one carbon neutron, or approximately 1.00335 AMU. The height of the M+1 and M-1 peaks differ directly according to the number of carbons in a molecule. For arginine, the heights of M+1 and M-1 are 32% the height of their respective monoisotopic peaks, representing a six-carbon molecule. The relative height of the M+1, the relative height of M-1, and the distance between the monoisotopic peaks all provide confirmation of the number of carbons = **triply redundant quality control** measurements.

Matrix is analyzed by LC-MS and ClusterFinder™ software to build a "dictionary" of RT, m/z, formula, and physiochemical characteristics:

- Triply redundant measurements ensure that the dictionary is both reproducible and accurate and allow algorithms to go deep into the noise to find compounds.
- Isotopic signatures in the compounds are mathematically calculable enabling algorithms to characterize peaks (artefacts, or Matrix compounds), remove unlabeled artefacts, calculate carbon number and molecular formula.
- Collected for every Matrix IROA peak is information from **primary scan** - i.e. retention time, ^{12}C and ^{13}C monoisotopic masses, number of carbons in the molecule; **in-source and post-source fragmentation** – i.e., orthogonal data from analyses including Ion Mobility, SWATH fragmentation, etc.
- Information is used to find these same features in experimental samples.
- Features monitored daily for any changes; the basis of instrument performance.

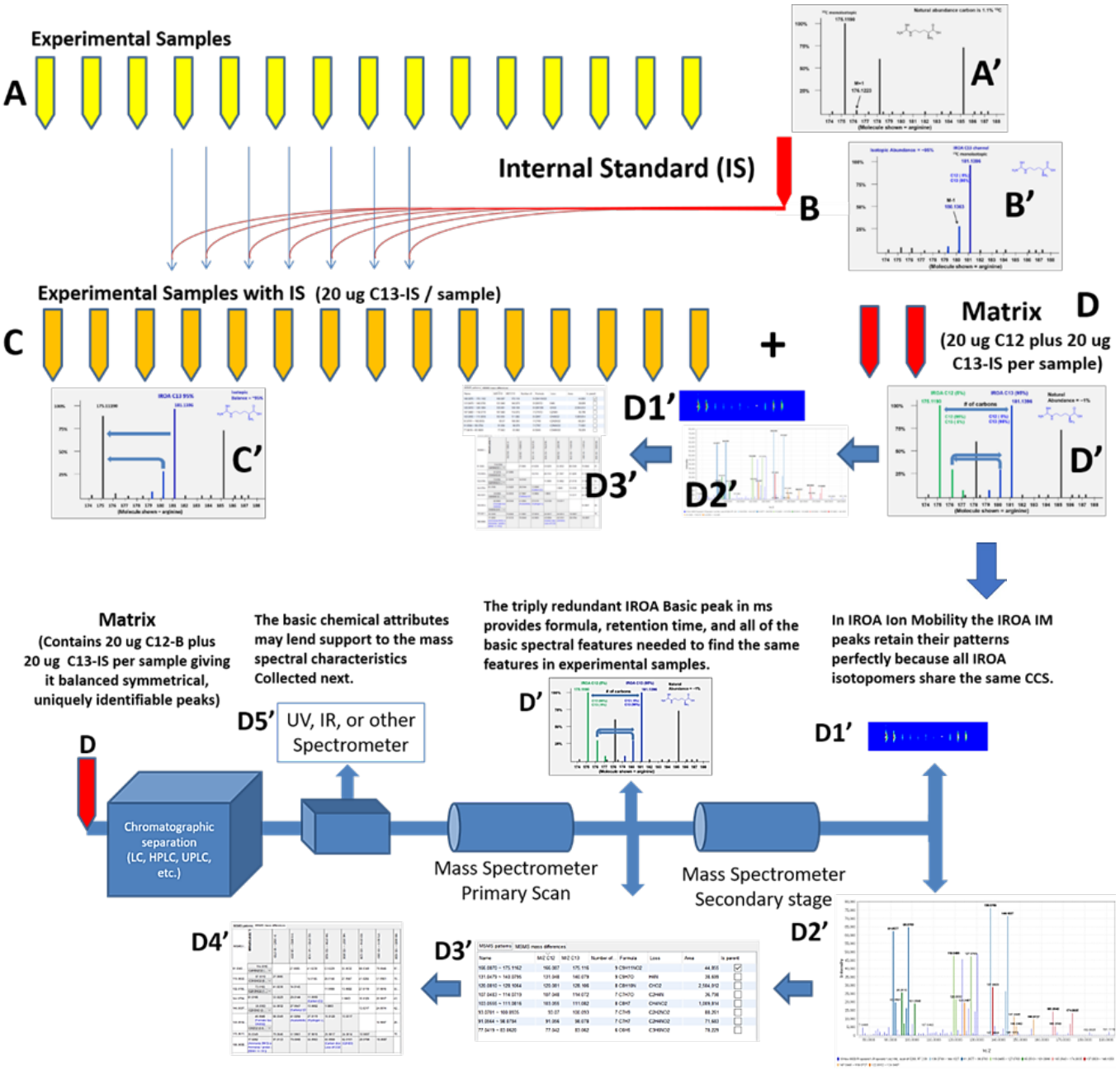

Figure 2. Experimental samples (A) contain compounds where the isotopic balance is present only at natural abundance, i.e. 1.1% ^{13}C (A'). A fully labeled 95% ^{13}C Internal Standard IS (B') is added to experimental samples. Experimental/IS samples and Matrix (D; fully labeled 95% and 5% ^{13}C, mixed 1:1) are randomly interspersed into a single sample set (e.g. one Matrix injection for every 10 experimental/IS samples) and analyzed using LC-MS. The same 95% 13C isotopomeric IROA signal is present in both the Matrix (D) and experimental/IS samples (C) and the chromatography is consistent across both, the Matrix is mapped directly to the experimental samples. The catalog of IROA peaks found in each daily Matrix analysis (D') provides a mechanism for correcting instrument error. Since the amount of IS is identical to that in the Matrix and is the same across all samples, the sum of all signals in the IS is constant and may be used to normalize samples. Natural abundance peaks are easily located and quantitated as they co-locate with their corresponding IROA peaks (C). In IROA MSMS fragmentation such as SWATH (D2') the IROA peaks retain their patterns (D3') because wide windows are used. Since all fragments retain their IROA character, their formulae (D4') and their relationships between them are determinable (D5'). With the inclusion of second stage analysis (D1-D5) the compounds found in the Matrix samples run under different analytical conditions i.e. HPLC system 1 and HPLC system 2, may be unequivocally mapped from one to the other and will provide for the quantitative comparison of experimental samples associated with their respective Matrix.

Matrix and IS identify compounds in experimental samples:

- Experimental samples are spiked with IROA **Internal Standard (IS)** – the same 95% U-^{13}C component of the Matrix, and at the same concentration.
- Experimental/IS samples and Matrix are randomly interspersed (e.g., one Matrix injection per 10 experimental/IS samples) and analyzed using LC-MS, **Figure 2.** The concentration of the compounds in Matrix and IS and their chromatography are identical.
- The software uses the information stored in the Matrix dictionary to identify where each of these same IROA peaks will be found in the experimental samples using the IS.
- The IS "yardstick" provides enough information for complete identification and quantitation of samples without the need for chromatographic base-line correction or using the same orthogonal identification system in the experimental samples (critical because secondary systems may lower temporal resolution and thereby lower the precision of the analytical measurement).
- Experimental natural abundance peaks co-locate with their corresponding IROA-IS peaks at a mass that is the mass of the IROA ^{13}C monoisotopic peak less the number of carbons it contains times the mass of a neutron.

During LC-MS, a metabolite is seen multiple times as neutral loss fragments of structurally-related parents due to in-source fragmentation. Post-source fragmentation also occurs using SWATH and other MSMS techniques. IROA-formatted peaks maintain their integrity through MSMS; fragments show as IROA fragmentation, and similarly through IM where all the IROA-peaks share a common CCS. Because fragments share the same unique IROA isotopic signatures as their parent compounds, ClusterFinder peak correlation analysis associates both in- and post-source fragmentation sets, greatly aiding in peak identification.

When analyzed, each Matrix has a library of validated compounds associated with it. Given the diversity of possible chemical structures, standard mass spectral data generated after chromatographic separation alone is not sufficient to identify most compounds, nor usually sufficient to identify a unique molecular formula. The monoisotopic mass and exact number of carbons in the molecule are known for all IROA peaks, and this is sufficient to provide a unique molecular formula. A molecular formula may be shared by a number of compounds, so while IROA provides assured formula it does not alone provide assured identification.

If in addition to the molecular formula for each IROA peak, we add collisional cross-section (CCS from IM), Fragmentation data (MSMS from SWATH, etc.), UV, IR, or other physical characteristic of each compound as determined in the Matrix sample and associated library of compounds, then the combination of assured molecular formula and these physical attributes become unique identifiers for each compound. This information is added to the "dictionary" and becomes the basis of completely reproducible accurate identification and quantitation, and the Matrix sample provides complete QA-QC of instrument performance on a daily basis.

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THE AUSTRALIAN & NEW ZEALAND METABOLOMICS CONFERENCE 2018

30 AUG - 1 SEP 2018
UNIVERSITY OF AUCKLAND

FEATURING:
'Introduction to Metabolomics' Lecture Series !

Dr Janine Cooney
The New Zealand Institute for Plant and Food Research Ltd

Prof Ute Roessner
University of Melbourne, AUS

Dr Horst Schirra
University of Queensland, AUS

A/Prof Sanjay Swarup
National University of Singapore, SG

A/Prof Silas Villas-Boas
University of Auckland, NZ

Prof David Wishart
University of Alberta, CAN

Friday June 1st 2018
Early Bird, Abstract & Rapid Fire Deadlines

ANZMET

www.anzmet.org

Recent Publications

Recently published papers in metabolomics

- Recent Advances in Targeted and Untargeted Metabolomics by NMR and MS/NMR Methods
- Metabolomics reveals perturbations in endometrium and serum of minimal and mild endometriosis
- Combined use of isotopic fingerprint and metabolomics analysis for the authentication of saw palmetto (Serenoa repens) extracts
- Metabolomics Based Dietary Biomarkers in Nutritional Epidemiology - Current Status and Future Opportunities
- MetaBridge: Enabling Network-Based Integrative Analysis via Direct Protein Interactors of Metabolites
- Multiplatform Metabolomics Investigation of Anti-Adipogenic Effects on 3T3-L1 Adipocytes by a Potent Diarylheptanoid
- Multiomics biomarkers for the prediction of nonalcoholic fatty liver disease severity
- Coupling MALDI-TOF mass spectrometry protein and specialized metabolite analyses to rapidly discriminate bacterial function
- Metabolomics approach to reduce the Crabtree effect in continuous culture of Saccharomyces cerevisiae
- Advances in Nutritional Metabolomics
- Targeted biochemical profiling of brain from Huntington's disease patients reveals novel metabolic pathways of interest

Metabolomics Events

BIRMINGHAM METABOLOMICS TRAINING CENTRE

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.

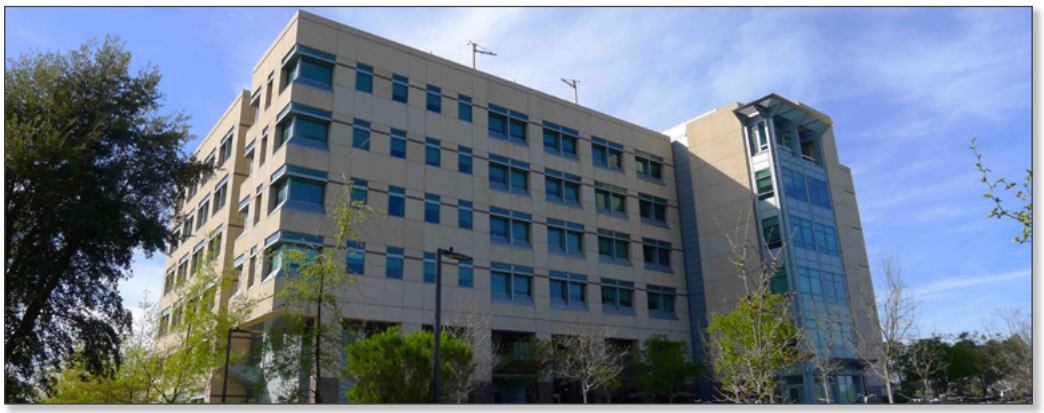
This workshop is free of charge and it will include the use of the MINE Database and tools as well as other cheminformatics and bioinformatics programs instrumental to biochemists, physiologists, and biologists working in metabolism.

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

BIRMINGHAM METABOLOMICS TRAINING CENTRE

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

THE UNIVERSITY of WISCONSIN MADISON

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

26-28 Aug 2018

1st Nordic Metabolomics Conference

Venue:
Aula Nova, Örebro University, Sweden

Welcome to the 1st Nordic Metabolomics Conference, which is the inaugural annual meeting of the newly established Nordic Metabolomics Society.

The conference aims to highlight and discuss the latest metabolomics research in Nordic countries and abroad. The meeting will start with a welcome reception in the evening of Sunday, August 26th and end in the afternoon of August 28th. The meeting will also host the 1st General Assembly of the Nordic Metabolomics Society.

Most of the talks for the conference programme will be selected from the submitted abstracts.

Key dates and information

- Registration and abstract submission opens: March 1st, 2018
- Deadline for early bird registration: June 30th, 2018
- Abstract submission deadline: May 14th, 2018 (for poster abstracts, submission for oral abstracts is closed)
- Final programme posted: May 31st, 2018
- Over 15 travel awards of 5000 SEK will be available, supported by the Örebro University and the Nordic Metabolomics Society. You can apply for the award as apart of the abstract submission process. Eligibility: student or postdoc, with submitted abstract.

For more information, visit https://www.oru.se/english/about-us/conferences/nordic-metabolomics-conference/.

27-31 Aug 2018

Introduction to Ecometabolomics for Ecologists

Venue:
Institute of integrative biodiversity research (iDiv), Leipzig, Germany

- When: 27-31 August 2018 (full day)
- Cost: No participation fees; only travel and hotel costs
- Content: lectures, discussions, student presentations; hands on: sampling, laboratory experiments, data analysis

The course will provide an overview about the application of metabolomics in ecological and biodiversity research. We will explore the tools and approaches that are used to obtain, process, and analyse metabolomics data. The course will be delivered using a combination of lectures, computer-based practical sessions with test data sets, group discussions, and hands-on practical exercises in the lab. Especially PhD students who are interested in performing or already plan to implement metabolomic analysis for their ecological and biodiversity research are invited.

Where can I apply?

For Application please contact: Henriette.uthe@idiv.de. Please add a short letter about why you want to take part in this course and what you expect to learn.

Furthermore, we will award two grants to cover travel and hotel costs. Don't hesitate to contact Henriette Uthe for more Information.

Deadline for application: 1 July 2018

For further information and registrations details, please visit https://www.idiv.de/ydiv/courses_and_training/introduction_to_ecometabolomics_for_ecologists.html

30 Aug - 1 September 2018

The Australian & New Zealand Metabolomics Conference

Venue:
University of Auckland, New Zealand

Featuring: **The Introduction to Metabolomics Lecture Series !**

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 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/.

BIRMINGHAM METABOLOMICS TRAINING CENTRE

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

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

Metabolomics Events

SardegnaRicerche

1-5 Oct 2018

4th Metabolomics Sardinian Summer School: "Nutritional Metabolomics"

Venue:
Polaris Technology Park, Pula, Sardinia, Italy

Course Objectives and Targets
Participants will attend theoretical sessions with lectures by experts, and hands-on data analysis aimed to deepen the theoretical and practical knowledge for using the main tools available to better understand the role of nutrition in health and disease. The School is mainly targeted to researchers at an early stage in their career (but not only), from Biological Sciences, Health Sciences and other different background (including bioinformatics) who are interested in learning about both technical and bioinformatics tools to be applied on Nutritional Metabolomics

Participants will learn about:
- How to design a metabolomics experiment;
- How to measure nutritional and metabolism biomarkers;
- How to find correlations between dietary habits and health.

Main Topics
- NMR and MS in Foodomics and Nutrition
- Ion Mobility techniques in lipids analysis.
- Statistics, Data fusion and Data integration
- Metabolomics, Microbiome and Nutrition
- Metabolomics: beyond biomarkers and towards mechanisms
- New challenges in Human Nutrition
- Lipidomics in Nutrition

Daily lectures and hands-on sections, plus poster and oral presentations from participants

Applications
The course is funded by the Regional Sardinian government and registration will be free of charge for all attendees. Selection will be based on CV and a letter stating the motivations for attending the course and future research plans of candidates. A letter of reference from the current supervisor must also be attached to the application. Registration includes course material, lunches and coffee breaks (not accommodation expenses). For selected participants contribution or reimbursement will be considered.

Organizing Committee
- Atzori Luigi, Università Cagliari, Cagliari, Italy (latzori@unica.it)
- Caboni PierLuigi, University of Cagliari, Italy (caboni@unica.it)
- Griffin Jules, University of Cambridge, Cambridge, UK (jlg40@cam.ac.uk)
- Pieroni Enrico, CRS4, Pula, Italy (ep@crs4.it)

Summer School Secretariat: nutrimet2018@gmail.com

For detailed information about the Summer School in Sardinia, visit:
Nutritional Metabolomics School 2018.

Metabolomics Events

8-12 Oct 2018

Workflow4Experimenters 2018 Course:
Analyze your LCMS, GCMS and NMR data with Galaxy and the Workflow4Metabolomics online platform

Venue:
Paris, France

During this "Bring Your Own Data" one-week course at the center of Paris (France), you will use Galaxy and the Workflow4Metabolomics online platform (W4M) to analyze your own LC-MS, GC-MS, or NMR data set. Morning sessions will be dedicated to methodology and tools. Afternoon sessions will be devoted to tutoring on your data.

Invited speakers: Christoph Steinbeck (Friedrich Schiller University - Jena) and Julien Boccard (University of Geneva)

Organization: Infrastructures for bioinformatics (ELIXIR-FR, IFB) and metabolomics (MetaboHUB).

Registrations: http://workflow4metabolomics.org
Contact: contact@workflow4metabolomics.org

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

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

Metabolomics Events

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

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.

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 in High-Throughput Metabolomics	Karolinska Institute International Open Laboratory	Maebashi, Japan	18-May-18	Until filled	Gunma University
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***