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

Metabolomics Society News

Conference Corner

Dear Colleagues and Metabolomics Enthusiasts,

As we write this, it is now 4 months to **Metabolomics 2021 Online**, and, on behalf of the Metabolomics Society, we would like to cordially invite you to Metabolomics 2021 Online, the 17th Annual Conference of the Metabolomics Society. The conference will run from Tuesday, June 22 to Thursday, June 24, 2021, and will have a fantastic program.

On day 1, there will be a series of exciting Workshops plus several Sponsor Studios. Days 2 and 3 of the conference will be the scientific program packed full with talks and other events:

- There will be a variety of scientific presentations, ranging from invited Keynotes, presentations promoted from abstracts, short flash talks, and informative industry talks.
- We aim to invite 12 exciting, diverse Keynote speakers.
- Don't forget the special events organised by the Metabolomics Society, e.g., the Town Hall Meeting with the reports/news from the leadership, special updates from the Early-Career Member Network and Membership Committees, etc.
- The Poster Gallery will be available 2 weeks before the conference, and will remain online during the event, giving you plenty of time to browse and ask questions to the presenter.

Talks are organized in three thematic streams: Health, Technology, and Environment, meaning there will be interesting science for everyone. As last year, the agenda will run in the "Live Aid" model with sessions around the clock, so that you will be able to access the meeting conveniently from your geographical region. In addition, presentations will be recorded and available within 2 hours following each session, so you do not have to get up in the middle of the night to watch your favorite session.

We're excited to enhance the EventsAir platform and have improved the features for socializing and networking, e.g., more engagement with our valuable sponsors in the virtual exhibit hall, easy ways to find and connect with other attendees in your same area of research, a newly designed poster gallery, and more to come!

Last year, the conference was free for Society members, to provide an anchor point for the community in the deepest depth of the pandemic and national lockdowns. However, **Metabolomics 2021 Online** is a complete conference with all the features and benefits that you've come to expect from us, and it costs the Society considerable effort/funds to put on a virtual conference of this scale. As such we are charging registration fees this year (similar to all other online conferences). Our fees are modest compared to the in-person meetings of the Metabolomics Society. We're working to bring you a robust agenda with new engagement opportunities, all a wonderful value! All current members of the Society (at the time of registration) will receive discounted conference registration fees.





METABOLOMICS SOCIETY EARLY- CAREER MEMBERS NETWORK

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

General Enquiries info@metabolomicssociety.org Membership Enquiries Metabolomics 2021 Online is your unique chance to connect to everyone in this second year of the pandemic and experience metabolomics surrounded by friends and colleagues. Come join us! Register online to reserve your space, as space is limited. Abstract submission is well underway, oral abstracts are **due April 7** and poster abstracts are due May 7.

For more updates on the conference stay tuned for the next issues for MetaboNews and the email announcements of the Metabolomics Society. Visit us at <u>www.</u> <u>metabolomics2021.org</u>.

We are looking forward to seeing you all at Metabolomics 2021 Online.

Horst Joachim Schirra Chair, Metabolomics Society Conference Committee

Members Corner

Board of Directors

Dear Colleagues,

We are excited to announce that registration is now open for the second virtual conference, Metabolomics 2021 Online, that will take place from June 22-24, 2021. The conference website is available at <u>www.metabolomics2021.org</u>. Similar to last year, the conference will take place in all time zones, enabling it to continue as a truly international event. Abstract submissions are now open! We welcome oral abstract submissions through April 7, 2021 and poster presentations until May 7, 2021. We will announce the selected oral talks in mid-May, please submit your latest cutting-edge work. We will also be announcing the Keynote speakers shortly, so please check back to see this year's line-up of interesting speakers.

In other Society news, we are excited to announce that we have started a Diversity, Equity, and Inclusion (DEI) Task Group, to help the Society best identify and address the important issues in this area. If you have experience and would like to contribute your expertise, please contact Natasa Giallourou (<u>natasagiallourou@gmail.com</u>) who is leading this effort.

We are also excited to announce the success of the Single Cell Metabolomics Workshop that took place in late February and had over 500 attendees! Please be on the lookout as we are looking forward to offering more virtual events throughout the year, with the hope of raising the quality of metabolomics research worldwide.

All the best,

Jessica ann Lacky-Su

Jessica Lasky-Su, President, Metabolomics Society





www.chenomx.com

Early-career Members Network (EMN)

EMN Award 2021

The EMN is delighted to announce the opening of the EMN Award for 2021. This award aims to encourage active engagement in the field by supporting and recognizing outstanding achievements, offering more visibility and great prices to the awardees.

Are you a graduate student or an early-career researcher? Are you planning to submit an abstract for the Metabolomics 2021 Online conference?



Then most of the job is already done! <u>Click here</u> to know more about the submission process and the prices.

EMN Webinar Series

Mark your calendars! The next Webinar organized by the EMN will be hosted on March 22nd 2021, at 14:00 UTC. The EMN is looking forward to welcoming Prof. Assaf Vardi and Dr Guy Schleyer, who will present how they utilize the recent advances in the field of chemical ecology (metabolomics and mass spectrometry imaging) combined with single-cell imaging and transcriptomic approaches to track host-pathogen interactions at the microscale. Click here to register!

New Expert Opinion

The new Expert Opinion is now published on the EMN wiki page, and it is a real pleasure to read the inspiring answers from Prof. Roy Goodacre, who shared his work and his experiences with us. <u>Follow the link</u> to find out more.

Membership News for 2021

A reminder that the Metabolomics Society is now offering a rolling-year membership, meaning your membership does not expire on December 31. Instead, it's valid for one year from the date of sign-up. If your membership is still active over the June conference dates, you'll receive discounted registration! Questions regarding membership can be directed to info@metabolomicssociety.org.

Task Groups Corner

NEW! Diversity, Equity and Inclusion Task Group Diversity equity and inclusion in the Metabolomics Society

Recognizing that discrimination racism and other forms of



structural inequality are widespread issues in science, the Metabolomics Society is committed to increasing diversity in our field by implementing diversity and inclusion into our activities and organisational culture. Productive, innovative and impactful scientific communities depend on rich diversity of perspectives, backgrounds and experiences. The Metabolomics Society feels there is a need to have a dedicated Task Group focused on helping to further cultivate a community where all members of feel welcome and secure and that all voices are heard and respected.

The purpose of this task group is to develop and promote strategies and best practices within the realms of racial, social sexual and gender diversity. We welcome participation from all members of the Metabolomics Society. If you are interested in getting involved, please contact Natasa Giallourou (natasagiallourou@gmail.com).

NEW! Best Practice and Essential Reporting Standards for Data Analysis

Announcement of New Task Group: Best Practice and Essential Reporting Standards for Data Analysis in Metabolomics

It has been well documented that there is a reproducibility crisis in science in general. Closer to home, there are areas of ambiguity within the data analysis pipeline for metabolomics. This is often not deliberate and can be, but not limited to, a lack of transparency in the reporting of the data analysis process, or the employment of push-button 'black box' automated approaches, compounded with a lack of user knowledge.

The Metabolomics Society has therefore created this task group to help establish best practices and recommendations for what needs to be reported in order to ensure reproducibility of metabolomics data analysis science. We believe this will have a positive impact and improve data analysis practices more broadly.

If you are interested in getting involved, please contact Roy Goodacre (<u>roy.goodacre@liverpool.ac.uk</u>).

International Affiliates Corner

Metabolomics Association of North America (MANA) Visit <u>https://metabolomicsna.org</u>

The hosts of MANA 2021 have been diligently preparing for the association's annual meeting!

Due to continuing uncertainties regarding the timeline of resolution of the COVID pandemic and institutional policies regarding travel, the decision has been made to hold MANA 2021 virtually. The meeting will occur over four days this year (October 18-21, 2021) and will include a day for preconference instructional workshops. As additional bonus material this year, there will be early morning sessions devoted to metabolomics and mass spectrometry called "Mass Spec Mornings", and that will occur before the main conference start time of 11:00 AM EST. These early morning sessions will be held in conjunction with the 2021 regional Ohio Mass Spectrometry and Metabolomics Symposium.

To stay up to date on the developing program, visit <u>MANA2021.org</u>, where you can also subscribe to ongoing updates.

We are looking forward to an exciting program!

Nordic Metabolomics Society Visit www.nordicmetsoc.org

The Metabolomics Society Precision Medicine Task Group in partnership with the Nordic Metabolomics Society, RFMF, and other organizations and interest groups is organizing a virtual workshop 'The Metabolome Meets the Exposome', to be held on Wednesday April 28, 2021 13:45 – 17:30 CET. https://www.nordicmetsoc.org/MetExposome2021.html

The Workshop will comprise invited talks and a general open discussion forum. Registration is free.

Other News

Call for Nominations: Honorary Fellows and Career Medals 2021

2021 Honorary Fellows of the Metabolomics Society

An Honorary Fellowship is a significant lifetime award granted by the Metabolomics Society to exceptional members of our community. Commissioned in 2012, and with up to two awards each year, the Board of Directors welcomes nominations from Members for these Fellowships, with a closing date of **April 8, 2021**.

See the <u>Honorary Fellowships website</u> for further details about the two categories of awards. Each nominee can be nominated for only one of the categories. The Board will consider only complete nomination packages, and these consist of the five items mentioned on the web page.



Metabolomics Society Career Medals

We are excited to continue the Society awards which seek to recognize the outstanding contributions of individuals to the field of metabolomics through the presentation of up to two Metabolomics Society Medals. These awards are open to all Society members who meet the eligibility criteria. While research contributions are of primary importance, other contributions, including to the teaching of metabolomics and/or service to the field or the society will also be strongly considered. There will be up to two medals awarded each year in the following categories:

- The Metabolomics Society Medal is for mid-career members of the Society and is open to those members who have been awarded a PhD 10-15 years prior to the closing date for nominations in each round. In 2021 this means your PHD must have been awarded between 2006 and 2011.
- **The President's Award** recognizes outstanding achievements in metabolomics. It is available for Society members who have been awarded a PhD no more than 5-10 years prior to the closing date for nominations in each round. In 2021 this means your PHD must have been awarded between 2011 and 2016.

See the <u>Metabolomics Society Career Medals website</u> for further details about awards. The application closing date is **April 8**, **2021**.





Metabo Interview | Dr. Emma Schymanski

Dr. Emma Schymanski



Head of the Environmental Cheminformatics Group at the Luxembourg Centre for Systems Biomedicine, University of Luxembourg

Short Biography

Associate Professor Emma Schymanski is head of the Environmental Cheminformatics (ECI) group at the Luxembourg Centre for Systems Biomedicine (LCSB), University of Luxembourg. In 2018 she received a Luxembourg National Research Fund (FNR) ATTRACT Fellowship to establish her group in Luxembourg, following a 6-year postdoc at Eawag, the Swiss Federal Institute of Aquatic Science and Technology and a PhD at UFZ - Helmholtz Centre for Environmental Research, Leipzig, Germany. Before undertaking her PhD, she worked as a consulting environmental engineer in Perth, Australia. She has over 80 publications and a book and is involved in many collaborative software efforts. Her research combines cheminformatics and computational (high resolution) mass spectrometry approaches to elucidate the unknowns in complex samples, primarily with non-target screening, and relating these to environmental causes of disease. An advocate for open science, she is involved in and organizes several European and worldwide activities to improve the exchange of data, information, and ideas between scientists to push progress in this field, including NORMAN Network activities (e.g., NORMAN-SLE), <u>MassBank, MetFrag</u> and <u>PubChemLite for Exposomics</u>.

Interview Q&A

How did you get involved in metabolomics?

I think we have to "blame" Steffen Neumann for my involvement in metabolomics. We first met now over 10 years ago at a workshop in Leipzig where he presented <u>MassBank (IPB)</u>, while I was still a PhD student at UFZ. We started collaborating on MetFrag almost instantly, then on MassBank.EU, then CASMI ... we celebrated our 10 years of collaboration virtually together with our families last year. Another key event was the Metabolomics Society meeting (and hackathon) in San Francisco in 2015, where I first met many of the international metabolomics world. Although for many years I claimed that I did not really "do" metabolomics, with my move to Luxembourg I now "do" and teach metabolomics, although with my environmental chemistry background, exposomics is currently earning more of our research attention as it combines "the best of both worlds" for me and presents many interesting challenges.

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

The people, the collaborations and seeing so many new and exciting open computational developments evolve because people are working together across the globe to solve problems to help make metabolomics easier for people to do. I like working with students and scientists on a wide variety of use cases (problems) and help them derive the answers from the data ... or see where this is not possible yet and point them to other methods that may help or try to improve our methods so that they can. I really enjoy working with major resources to help improve things for our use cases, and seeing the new de-



Metabo Interview | Dr. Emma Schymanski

velopments "go live" for the benefit of all.

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

At the moment we are heavily focused on cheminformatics and data initiatives to help make non-target (or untargeted!) exposomics and thus also metabolomics easier. Identification in non-target experiments requires the connection of a lot of different data streams, we work on improving these connections and, more critically for where the field currently stands, on how to improve the interpretation of the data for end users (no mean feat in an exposomics context). Rick Helmus' work on patRoon is a prime example of a very comprehensive open mass spectrometry workflow system in R (building on many other open initiatives) that is under continual development as users apply it in their dayto-day work. Our **PubChemLite for Exposomics** collection, I believe, is an important step in being able to both define a dynamic and relevant chemical space for various studies and offer improved interpretation by leveraging the rich annotation content in PubChem, which is transferable to other resources. With our in-house approach Shinyscreen we are both trying out new approaches to data analysis and teaching young scientists how to design interfaces (designed by students for students).

What is happening in your country in terms of metabolomics?

Even though Luxembourg is a small country, we are very active in metabolomics. My neighbouring PI Carole Linster heads the Enzymology and Metabolism group and runs the Metabolomics Platform. Since she is largely experimental and I am largely computational, this is a highly complementary and very beneficial overlap for both groups. Both the University (including LCSB, where we are and <u>FSTM</u>) and the Luxembourg Institute for Health (LIH) have many researchers that use metabolomics initiatives; for example, Paul Wilmes, Johannes Meiser and Elisabeth Letellier are regular users of the platform. We have a very strong **Bioinformatics Core**, and I enjoy working especially with the <u>R3 team</u> on reproducible, responsible (open) research. Being so geographically small, we reach out to our neighbours a lot, e.g., the YoungNMC network in BeNeLux (Belgium, Netherlands, Luxembourg) for young scientists and students, and I like to teach or participate in European events to keep the ties going, e.g., France (RFMF Toulouse Jan. 2020), Germany (metaRbolomics), Belgium, ELIXIR ... the list goes on ... they often say Luxembourg is the "heart of Europe" and it seems to be the case!

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

I see our work being applied in many efforts, both with students and collaborators, and more importantly beyond. I keep an eye on what people find useful and really enjoy seeing others benefit from our developments or take what we do and develop it further! I take feedback and expressions of interest on board and use this to help drive our next developments. I would hope that we in research maintain the freedom and ability to try out new ideas and approaches, and that the best ones are picked up and made available to a much wider range of users through a variety of platforms. It's one of the big motivating factors for me to do open science.

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

I really like this quote from Blaženovic et al. 2018, DOI: 10.3390/metabo8020031 "The computational metabolomics community is small but innovative ... groups worldwide contribute in friendly competition" - we work with each other, integrating our resources wherever possible, yet still finding our respective niches to perform innovative work. This "friendly competition", as long as it remains friendly, is really the great strength. I believe we will need a variety of open resources, as different scientists interact differently with them, and have an enormous range of questions to be answered that require vastly different expertise - I use plenty of tools and resources beyond those that we develop. There is so much to do, and so little time in which to do it, that we are much stronger working together to achieve great things while giving each other the space needed for individual efforts – bearing in mind of course that we are all human and there are still only 24 hours in the day, and this is never enough!

What do you see as the greatest barriers for metabolomics?

... anything that hinders the above.

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

I would say metabolomics has taken off ... we now need to keep it flying (higher). To keep flying, I believe we need to be able to maintain and develop the key international open resources upon which much of the metabolomics in research is based. It's nice to see such funding initiatives start, e.g., the <u>NIH Common Fund Metabolomics</u>, but such support will need to continue. Maintaining open software and databases is an extremely resource intensive exercise that many underestimate.



Metabo Interview | Dr. Emma Schymanski

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

Locally, health and the environment are priority research areas for Luxembourg and thus there are many opportunities available through the Luxembourg National Research Fund (FNR), also opportunities on the European level, although recent interest in our group has come primarily from the environmental and exposomics side! I find it concerning that funding cycles are so short, whereas a lot of the data and computational infrastructure needed involve long term investments and maintenance to allow stability and constant updating to be "state-of-the-art", without having to introduce completely new resources as "novel research". I have been very fortunate that the FNR provided me the funds to develop what we currently do; we would not have been able to launch so many computational initiatives in such a short time without their support.

What role can metabolomics standards play?

I think standards can and will play a vital role in applying metabolomics (and eventually exposomics) in a more routine setting. A degree of standardization and comparability across the globe will be needed to transform this from a single-lab endeavour to a truly global endeavour with e.g., comparable cohort analysis and reporting across multiple labs using a carefully designed and selected subset of standard methods. This will also enable the development of more standardized data analysis methods rather than tailor made solutions. On the other hand, while embracing the move to standardization for some research questions where this is certainly needed, a certain degree of flexibility must also remain to be able to perform cutting-edge research and push the boundaries of the possible. It's a difficult set of compromises to find.

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

There are possibly some people reading this whose work I greatly admire and who have helped shape what we have become and what we do today. There are many who are not even mentioned, either directly or indirectly, not to mention some of the future generation who may be starting small but will help shape metabolomics now and into the future. Thus, my closing remark would be for all of you to keep up the great work and to say thanks to all of you for your contributions and interest!



Recent Publications

Recently published papers in metabolomics

- <u>The maternal serum metabolome by multisegment injection-capillary electrophoresis-mass</u> <u>spectrometry: a high-throughput platform and standardized data workflow for large-scale</u> <u>epidemiological studies</u>
 - For a "behind the paper look" at this study, check out <u>this blog</u> by TMIC Node Leader <u>Philip Britz-McKibbin</u>.
- <u>A Multi-Platform Metabolomics Approach Identifies Urinary Metabolite Signatures That</u> <u>Differentiate Ketotic From Healthy Dairy Cows</u>
- Metabolomic evaluation of serum metabolites of geese reared at different stocking densities
- <u>MALDI matrices for the analysis of low molecular weight compounds: Rational design, challenges</u> <u>and perspectives</u>
- <u>Targeted metabolomics as a tool for the early diagnosis of Diabetic Kidney Disease in Type II</u> <u>Diabetes Mellitus patients</u>
- Spatially Resolved Mass Spectrometry at the Single Cell: Recent Innovations in Proteomics and <u>Metabolomics</u>
- <u>Metabolic signatures of osteoarthritis in urine using liquid chromatography-high resolution</u> <u>tandem mass spectrometry</u>
- <u>Comprehensive evaluation of the metabolic effects of porcine CRTC3 overexpression on</u> <u>subcutaneous adipocytes with metabolomic and transcriptomic analyses</u>
- Role of the oral microbiome, metabolic pathways, and novel diagnostic tools in intra-oral halitosis: a comprehensive update
- <u>Oral administration of *Akkermansia muciniphila* elevates systemic antiaging and anticancer <u>metabolites</u></u>
- Metabolomics and lipidomics in *C. elegans* using a single sample preparation
- Mass spectrometry-based metabolomics diagnostics myth or reality?
- <u>An elaborative NMR based plasma metabolomics study revealed metabolic derangements in patients with mild cognitive impairment: a study on north Indian population</u>

Postponed Until 2021

The Third Annual Canadian Metabolomics Conference

Venue

Edmonton, Alberta, Canada

Overview

The Third Annual Canadian Metabolomics Conference has been postponed until 2021. The conference will highlight work by leading researchers, including new technologies and approaches for metabolomics research, and applications in various fields. The conference will feature networking opportunities and a poster session designed for trainees to present their work. Our goal is to highlight the exceptional metabolomics science that is being done in Canada and abroad, and foster Canada's leadership role in the global research community.

We look forward to seeing you in 2021!

Conference Link https://www.canmetcon.ca/

8-26 March 2021

Quality Assurance & Quality Control in Metabolomics

Venue

Online, Birmingham Metabolomics Training Centre, University of Birmingham, UK

Overview

The application of quality assurance and quality control in the metabolomics field is vital to ensure the collection of high quality data. In this course you will explore the importance of quality assurance and quality control in both untargeted and targeted metabolomics studies. We will explain the difference between quality control and quality assurance and how to apply in your studies and laboratories. You will evaluate the types of quality control samples that can be applied in metabolomics, what is the most appropriate quality control sample to use in your research, and how to apply the data in your quality assurance procedure to produce robust and reproducible data.



Topics Covered

- What are quality assurance and quality control and how do they differ
- What is the importance of quality assurance in metabolomics
- The types of quality assurance and quality control in untargeted and targeted metabolomics
- The importance of quality control samples
- The types of quality control samples applied in untargeted and targeted metabolomics
- Preparation of quality control samples in untargeted and targeted metabolomics
- Analytical studies including untargeted and targeted metabolomics
- Processing data in untargeted and targeted metabolomics
- Recommended quality assurance procedures in untargeted and targeted metabolomics
- Reporting quality assurance procedures in untargeted and targeted metabolomics

Course Link

1 April 2021

Introduction to Bayesian Statistics in Metabolomics

Venue

Online, University of California, Davis, California, USA

Instructor

Dr. Christopher Brydges, UC Davis

Registration

Required software:

• JASP (can be downloaded for free from <u>https://jasp-stats.org</u>). The current version is 0.14, but it may well be updated between now and April.

Participant prerequisites: Basic knowledge of statistics (e.g., know what a t-test and a correlation are). No coding experience needed, and there is no coding taught in this session.

Short description of the course: Bayesian statistics are a useful method for estimating effect sizes and testing the strength of evidence in favor one hypothesis over another—things that p-values and traditional statistics can't do. However, they are under-utilized in metabolomics research. This short course will provide a brief refresher on traditional statistics, teach the basic principles behind Bayesian statistics, learn how to conduct basic Bayesian analyses in JASP (free, open-source software available from https://jasp-stats.org/) and learn how to report the results in the style of a journal article.

For more information, please visit the Bits & Bites: Short Course Series 2021 website.

6-7 April 2021

Targeting CNS Tumor Metabolism Symposium

Venue

NIH Campus, Bethesda, Maryland

<u>Complimentary registration</u> thanks to the generosity of the Dabbiere Family. <u>View Program</u>



Overview

The SNO-NCI Joint Symposium: "Targeting CNS Tumor Metabolism" will foster collaboration in the area of metabolism which will positively influence outcomes for patients with CNS cancers. This is the first conference that focuses on the tumor metabolism and it is expected to be both didactic as well as a collegial learning environment with the goal to enhance partnerships and advance the treatment for patients. Metabolic investigations for these tumors have been conducted in isolation and the goal of this meeting is to bring together the clinicians with the experts in metabolism in order to increase the utilization of metabolic investigations in the clinical settings.

Participants will gain new understanding in CNS tumor metabolism via the use of state-of-the-art techniques; the interaction between the metabolism and the other -omics such as epigenomics, transcriptomics, as well as the current standard of care; and the challenges in targeting the metabolic signaling pathways.

Topics Covered

- Epigenome, Transcriptome, Metabolome and Modeling
- Metabolic Fluxes and Signaling of Metabolic Pathways
- New Technologies for Studying Brain Metabolism
- Metabolic Biomarkers and Imaging
- Metabolic Drug Targets, Resistance

Conference Link

15-16 Apr 2021

Data Analysis for Metabolomics

Venue

Wageningen Campus, The Netherlands

Overview

Metabolomics experiments based on mass spectrometry (MS) or nuclear magnetic resonance (NMR) produce large and complex data sets. This course will introduce approaches to process and analyze data and design high-quality experiments. Through hands-on workshops and lectures highlighting the different concepts you will get a thorough basis for tackling the challenges in metabolomics data analysis.

For information and registration, click here.

3 June 2021

Using MSDIAL to Generate Accurate Comprehensive LC-MS/MS Metabolomics Datasets

Venue

Online, University of California, Davis, Davis, California

Instructor

Jake Folz, University of California, Davis

Registration

Required software:

MS-DIAL vs. 4.0 for PCs. This software does not run on Mac or Linux environments.

Participant prerequisites: Basic understanding of LC-MS and understanding of how MS/MS spectra are used in metabolite identification.

Short description of the course: This short course will focus on how to perform fine tuned curation of processed LC-MS/MS data generated through MS-DIAL including compound identification, data quality analysis, and unknown feature reduction. Data from rat blood plasma analyzed using LC-MS/MS with MS/MS data collected in a data-dependent manner will be used to generate an example dataset, but the methods and techniques are applicable to many different sample types.

For more information, please visit the Bits & Bites: Short Course Series 2021 website.

15-18 June 2021

Hands-on Data Analysis for Metabolic Profiling

Venue

Online, Imperial College London, London, United Kingdom

Overview

This course will be run online, with Live lectures and tutorials using MS Teams.

We offer a comprehensive, hands-on training in processing and analysing metabolomics data from LC-MS and NMR technologies.

Attendees will have the opportunity to:

- Learn directly from internationally recognised leaders in the field
- Benefit from practical training in computational techniques and statistical methods

Course Aims

This 3.5 day online course provides a comprehensive overview of data analysis for metabolic profiling studies focussing on data from NMR spectroscopy and Liquid Chromatography-Mass Spectrometry. It combines lectures and tutorial sessions using open source software to ensure a thorough understanding of the theory and practical applications.

Course Link

22-24 June 2021

Metabolomics 2021 Online

Save the Date! Metabolomics 2021 Online will take place June 22 - 24, 2021. Registration is now open!

We are excited to introduce **Metabolomics 2021 Online**, the second virtual conference that will take place from June 22-24, 2021. While we will not be meeting in person, I am confident that the caliber of our program this year will push the boundaries of our understanding in multiple domains of metabolomics research.

The conference will follow the general format that we instituted for Metabolomics 2020 Online, with



the conference taking place in all time zones, enabling it to continue as a truly international event. We will open the conference with day 1 offering workshops on special interest topics, which has now become a tradition of our conference format. Days 2 and 3 will feature scientific sessions that will begin with a keynote speaker followed by talks selected from submitted abstracts and the ability for viewers to ask questions, in order to maximize member interactions. For each of us, some talks will be at more convenient times than others because the conference will take place through many time zones. Fortunately, recorded talks will be available to access and watch later during the virtual event, so don't worry about staying up all night to attend a talk you wanted to hear at 3 AM!

We will also host virtual poster sessions, networking opportunities, and special interest sessions that will include a town hall and early career member network meetings, among others. One thing that we can say is the plethora of virtual meetings over the last year has taught us much on how to effectively engage through virtual events and we will use this to our advantage. So get excited about Metabolomics 2021 Online! Registration fees for the meeting will be greatly reduced for all registered members of the Society.

Now is a great time to become a member of the Society! If you are already a member, then please go ahead and register for the meeting. I would also encourage you to submit an abstract to present your work at the conference, as we depend on each of you to hear about the latest in cutting-edge research. We look forward to seeing you virtually at Metabolomics 2021 Online.

Conference Link



22-24 June 2021

EMSL's 2021 Summer School

Institution

Pacific Northwest National Laboratory, Richland, Washington, USA

Environmental Molecular Sciences Laboratory

Extending the frontiers of biological and environmental science. EMSL provides world-class expertise and tools.

For more information, please visit the EMSL website.



5 Aug 2021

Identification of Unknown Compounds in Untargeted Metabolomics using Freely Available Software for Compound ID

Venue

Online, University of California, Davis, California, USA

Instructor Dr. Arpana Vaniya, UC Davis

Registration

Required software:

<u>MS-FINDER</u> & <u>SIRIUS+CSI:FingerID</u>. CFM-ID will be the web-based tool. Versions of tools to be used will be announced closer to the course date.

Participant prerequisites: Basic knowledge of computer skills. No coding experience needed.

Short description of the course: Compound identification is known as the bottleneck in metabolomics. However, there are many approaches one may consider while tackling this challenge (i.e., mass spectral library search, in silico fragmentation tools, or database searching). This short course will provide an overview on the current status of compound ID in metabolomics, participants will learn how to use some current tools for compound ID (i.e., CFM-ID, MS-FINDER, and SIRIUS+CSI:FingerID), and apply those skills to some unknown challenges.

For more information, please visit the Bits & Bites: Short Course Series 2021 website.

30 Aug-10 Sep 2021

International Summer Sessions in Metabolomics

Venue

Online, University of California, Davis, California, USA

Registration

The course will include:

- 1. Study design, including pitfall analysis and hidden biases in studies from microbial, plant, mouse and human cohort research
- 2. Sample preparation and quality control
- 3. In-laboratory detailed discussions standard operating procedures for GC-MS and LC-MS data acquisitions
- 4. Targeted metabolomics, including monitoring charts and use of isotope labeled internal standards
- 5. Exercises on flux analysis in cancer cells by isotope tracer analysis
- 6. Untargeted data processing and exercises on MS-DIAL software
- 7. Exercises on identification of unknowns by cheminformatics software workflows (incl MS-FINDER, CFM-ID, and various databases and small software routines)
- 8. Data normalization and transformation with and without internal standards and quality controls
- 9. Multivariate and univariate statistics
- 10. Pathway mapping

For information and registration click here.

17-19 Oct 2021

3rd Annual MANA Conference: Foods for Health Discovery Theme

Venue

The Ohio State University, Columbus, Ohio, USA

MANA 2021 conference website

If you seek to get *your* planned metabolomics event endorsed by MANA and receive MANA funds, please <u>contact us</u>!



Metabolomics Jobs

Metabolomics Jobs

If you have a job you would like posted, please email Ian Forsythe (metabolomics.innovation@gmail.com).

Jobs Offered

Job Title	Employer	Location	Posted	Closes	Source
Various Positions			16-Mar-21		<u>Metabolomics</u> <u>Association of North</u> <u>America Jobs</u>
UCD Post-doctoral Research Fellow Level 1	UCD	Dublin, Ireland	12-Mar-21	30-Apr-21	<u>MetaboNews Jobs</u>
Post-doctoral Fellow - Metabolomics via NMR, Neuro-Oncology Branch	National Cancer Institute	Bethesda, MD, USA	8-Mar-21	Until Filled	<u>National Cancer</u> <u>Institute</u>
Research Fellow in Computational Toxicology, Remote, with travel to partner locations in the United Kingdom required for specific project activities	University of Birmingham	Birmingham, UK	3-Mar-21	22-Mar-21	<u>University of</u> <u>Birmingham</u>
Postdoctoral Research Fellow, Metabolomics and Nutritional Epidemiology	McMaster University	Hamilton, ON, Canada	23-Feb-21	5-Jul-21	<u>TMIC Careers Page</u>
Marketing Specialist – Metabolomics Application Development (147595BR)	Thermo Fisher Scientific, Inc.	San Jose, California, USA	23-Feb-21	Until Filled	<u>Thermo Fisher</u> <u>Scientific, Inc.</u>
Marketing Specialist – Metabolomics Application Development (148431BR)	Thermo Fisher Scientific, Inc.	San Jose, California, USA	23-Feb-21	Until Filled	<u>Thermo Fisher</u> <u>Scientific, Inc.</u>
Research Technologist	Cold Spring Harbor Laboratory	Cold Spring Harbor, NY, USA	17-Jan-21	Until Filled	<u>Cold Spring Harbor</u> <u>Laboratory</u>
Post-doctoral Fellow / Staff Scientist – Metabolomics	Oklahoma Medical Research Foundation	Oklahoma City, Oklahoma, USA	17-Dec-20	Until Filled	<u>Metabolomics</u> <u>Society Jobs</u>
Postdoctoral Researcher in Analytical Environmental Cheminformatics	University of Luxembourg	Belval Campus, Luxembourg	Dec-20	Until Filled	<u>University of</u> <u>Luxembourg</u>



MARCH 2021

Metabolomics Jobs

Job Title	Employer	Location	Posted	Closes	Source
PhD Research Project Opportunities, Centre for Integrative Metabolomics and Computational Biology	Edith Cowan University	Joondalup, Australia	13-Dec-20	Until Filled	<u>Edith Cowan</u> <u>University</u>
Postdoctoral Scholarship - Metabolomics in Diabetes Research	Lund University	Lund, Sweden	24-Nov-20		<u>Lund University</u>
Postdoctoral Position	NIH	Rockville, Maryland, USA	20-Nov-20	Until Filled	<u>Metabolomics</u> <u>Society Jobs</u>
Post-Doctoral Position with influence of multiple 'omics' datatypes on the development of respiratory and/or neurological disease	Brigham and Women's Hospital and Harvard Medical School	Boston, MA, USA	20-Nov-20	31-May-21	<u>Metabolomics</u> <u>Society Jobs</u>
Postdoctoral Fellow – Biosensors Device Development	University of Alberta	Edmonton, Canada	23-Oct-20	Until Filled	<u>Wishart Research</u> <u>Group</u>
Postdoctoral Position in Nuclear Magnetic Resonance (NMR) Spectroscopy	University of Alberta	Edmonton, Canada	23-Oct-20	Until Filled	<u>Wishart Research</u> <u>Group</u>
Laboratory Assistant/ Technician – Biosensors Device Development	University of Alberta	Edmonton, Canada	23-Oct-20	Until Filled	Wishart Research Group
Senior Bioinformatician/ Cheminformatician Position	University of Alberta	Edmonton, Canada	23-Oct-20	Until Filled	<u>Wishart Research</u> <u>Group</u>

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 (<u>metabolomics.innovation@gmail.com</u>). Upon review, a limited number of job submissions will be selected for publication in the Jobs Wanted section.

• <u>Dr. Nara Consolo</u> - Seeking a position involving the application of NMR-based metabolomics in animals/animal production; it could be a Researcher position or an Assistant Professorship

