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mlowings@ualberta.ca <mlowings@ualberta.ca>
Reply-To: mlowings@ualberta.ca
To: metabolomics.innovation@gmail.com

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MetaboNews

This month in metabolomics

March, 2024
Vol 14, Issue 3

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

In This Issue

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Metabolomics Society News

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

General Enquiries

info@metabolomicssociety.org

Conference Corner

Join us in Japan, June 16-20, 2024, for plenary sessions, a busy exhibit hall with industry partners and a huge poster gallery, workshops, and over 25 scientific sessions!

Website: www.metabolomics2024.org
Hosted by: The Metabolomics Society
When: June 16-20, 2024

Conference Registration Open!

Conference registration is now open. Save money and register online before April 1 to receive the discounted early rate. Members receive an extra discount, so become a member of the Society before registering for the conference for savings!

Members' Corner

Board of Directors

Dear Society Members,
In fiction (Winston Groom in 1986) and film (who can forget Tom Hanks' Oscar performance in 1994) Mama Gump (played by Sally Field) once told Forrest that "Life is like a box of chocolates, you never know what you're gonna get!". It's true – life is full of surprises and like life, metabolomics (in the original untargeted version) is also complex, uncertain, and very often surprising. But rather than using the analogy of a box of chocolates, I think more of chicken tikka masala – a very popular dish in the UK (some may say our national dish!). This British dish was influenced by Indian cuisine and as well as containing chicken marinated in yogurt with spices (often garam masala, turmeric and cumin), this dish also includes onions, garlic and ginger. Now this is certainly complex and undefined, and I think metabolomics would currently fail to catalogue all the chemical

components, especially when one considers chirality and isomeric compounds which are vital to taste and texture of this very yummy spicy dish, yet analytically very challenging.

Despite this musing into food, every time we generate a metabolomic profile we are faced with the challenges of overcoming this complexity and making sense of the biological milieu we have just measured. A sensible estimate is that in metabolomics only 5% of the peaks – seen in a chromatography-based separation coupled with mass spectrometry – can be named with any degree of certainty. The likelihood is that many of these peaks are yet to be annotated and this so-called dark metabolome includes small (and large) molecules that have no reference structures, and also include things that are not detected at all (e.g., due to a lack of ionisation). The most concerning thing here (unlike the box of chocolates, which is finite) is that there is really no way to estimate the true size of this 'dark matter' within our metabolomics experiments.

With the above in mind, I am therefore very much looking forward to Metabolomics 2024 in Osaka and in particular to listening to our new Metabolomics Society Honorary Fellow Prof. Pieter Dorrestein from UC San Diego. Pieter and his team's work has focused on improving metabolite annotation and making these findings publicly available via GNPS, this will hopefully help in improving metabolite annotations and identifications.

I am also very much looking forward to listening to Prof Jules Griffin's plenary. Jules is also a very recent Metabolomics Society Honorary Fellow and he's based in the Rowett Institute and University of Aberdeen. This is reasonably close to the origins of the chicken tikka masala, which is purportedly to have been created in Glasgow! Jules will be talking on metabolomics within the metabolic syndrome and how nutrition plays a major role in human health. There's some joke in here about the Scottish diet and nutrition but it escapes me now… and I'm sure Jules will do a better job of enlightening us.

I'm also looking forward to our other plenary speakers:

- Prof Claudia Langenberg from Queen Mary University of London in UK whose work focuses on the genetic basis of metabolic control;
- Prof Kazuki Saito from the RIKEN Center for Sustainable Resource Science in Japan who works in plant metabolomics and phytochemical genomics; and
- Dr Yu Xia from Tsinghua University in China who has recently developed structural lipidomics tools which are capable of resolving structural isomers.

There are many other invited speakers and the conference agenda is starting to take shape and can be seen here: https://www.metabolomics2024.org

As you can tell I am getting excited about our Society's meeting in Japan. I'm excited

about the awesome science we shall discuss, as well as meeting old friends and making new acquaintances. I'll also be looking forward to tasting the Japanese cuisine and reminiscing on the last couple of times I visited Japan, which was in Tsuruoka in 2005 for our very first international meeting and again in 2014. I'm sure that some new happy memories will be made.

I hope your plans for Osaka and our 20th Annual Conference of the Metabolomics Society are going well. And I hope to see you soon.

All the very best.

Roy Goodacre, University of Liverpool, UK

President, Metabolomics Society

TODAY is the last day for registration and poster abstract submission!

The 5th Annual Canadian Metabolomics Conference (CanMetCon 2024), scheduled for Thursday, 25 April to Friday, 26 April 2024, at the Jack Poole Hall, The University of British Columbia, Vancouver, BC, co-hosted by The Metabolomics Innovation Centre (TMIC) and the UBC Department of Chemistry.

This year's conference is themed "Integrating Metabolomics with Other Omics", featuring four broad topics in the applications of Biological and Cellular Systems, Omics in Clinical Studies and Biomarker Discovery, Agricultural and Nutritional Applications, and Public

Health and the Epigenome.
More information about the program is available here

- Registration and Abstract for Poster Presentation Deadline: **March 22, 2024**

Registration fees are **CAD 150** for students and **CAD 250 plus applicable taxes and fees**. Your registration fee includes a welcome reception on April 25, breakfast and lunch on April 25–26, and light refreshments during morning and afternoon coffee breaks. See you in Vancouver!

Early-career Members Network (EMN)

EMN Webinar Committee- Webinars
The February webinar “Lipidomics workflows: from analysis to data integration” presented by Dr. Maria Fedorova is now available on the Metabolomics Society website. Dr. Fedorova discussed high-throughput LC-MS pipelines for tissue lipidomics and epilipidomics considering advanced bioanalytical and computational tools. Check the recording on https://metabolomicssociety.org/resources/multimedia/emn-webinars-2024/

EMN Conference Committee-MetaboArt Competition
This year, the EMN is again opening the MetaboArt competition to allow showcasing research projects in metabolomics through creative ideas. We strongly recommend the participation of scientists at any stage of their career as we strongly believe that images can be more effective than words in explaining scientific research. Both, members and non-members of the Society are welcome to participate. You do not have to attend the conference to be eligible. The winners of the MetaboART competition will be announced on June 10 on EMN Twitter.

EMN Networking Committee-Networking Event

Registrations are still open for the 2024 ECR Virtual Networking Event! This event, co-organized by the Metabolomics Society and the Metabolomics Association of North America (MANA), is scheduled for March 21st at 9:00 AM EST. Join us at https://bit.ly/ECRNetworking2024.

Task Groups' Corner

Lipidomics Task Group (LipidMet)

Upcoming LipidMet Meeting
March 26th 2024, 7 pm – 8:30 pm CET

Join Zoom Meeting
https://oru-se.zoom.us/j/65760856576?pwd=WndGTXJPRHB1Q1BZREFvemQwUklBUT09
Meeting ID: 657 6085 6576
Passcode: 659029

Agenda:

1. LipidMet updates in brief

2. Four 15-min talks on the theme of data deposition, standards, and reuse (discussion after all talks)
3. Discussion

The talks:

- Eoin Fahy, University of California San Diego/San Diego Computer Center, USA
  “The National Metabolomics Data Repository and integrated resources on the Metabolomics Workbench”
- Noemi Tejera Hernandez, EMBL-European Bioinformatics Institute (EBI), Hinxton, UK
  “MetaboLights: Database for metabolomics and lipidomics experiments and derived information”
- Pieter Dorrestein, Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, USA.
  “Reverse metabolomics - a big data lipid and metabolite discovery strategy”
- Nils Hoffmann, Institute for Bio- and Geosciences, Research Center Jülich GmbH, Jülich, Germany and Institute for Analytical Chemistry, University of Vienna, Austria
  “HUPO-PSI MS - An overview of data standards for mass spectrometry, current developments and how to get engaged”

International Affiliates' Corner

Polish Society of Metabolomics

Visit: https://ptmet.pl/

The Polish Proteomics Society and the Polish Society of Metabolomics invite you to a lecture titled "TMT-based quantitative MS analysis in mitochondrial maintenance studies." Enzo Scifo from the Translational Biogerontology Lab at the German Center for Neurodegenerative Diseases DZNE in Bonn will give the lecture.

The online event will be held on Thursday, April 11, 2024, at 4 pm CET via the TEAMS platform.
Meeting Details:

- Meeting ID: 365 986 665 954
- Passcode: XiDTpT

Please feel free to circulate the information among any colleagues who may be interested. We are looking forward to your participation.

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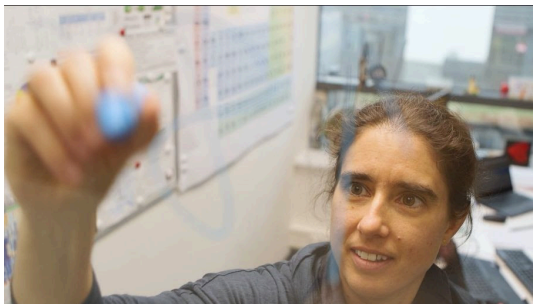
MetaboInterview

Emma Schymanski



Prof. Emma Schymanski
Head of the Environmental Cheminformatics Group
Luxembourg Centre for Systems Biomedicine (LCSB)
University of Luxembourg

Environmental Cheminformatics Group

Biography

Professor Emma Schymanski is head of the Environmental Cheminformatics (ECI) group at the Luxembourg Centre for Systems Biomedicine (LCSB), University of Luxembourg and special advisor to the rector for Open Science and Research Data Management. She became Full Professor in 2023, Associate Professor and Luxembourg National Research Fund (FNR) ATTRACT Fellow in 2018, following a 6 year postdoc at Eawag, Switzerland and a PhD at UFZ, Leipzig, Germany. Before her PhD she was a consulting environmental engineer in Perth, Australia and holds a double degree in Chemistry and Environmental Engineering from UWA, Australia. She is involved in many collaborative efforts, with over 100 publications and a book. Her research combines cheminformatics and computational (high resolution) mass spectrometry approaches to elucidate the unknowns in complex samples, primarily with non-target screening, and relate these to environmental causes of disease. An advocate for FAIR and open science, she is involved in, supervises 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 the NORMAN Suspect List Exchange (NORMAN-SLE), MassBank, MetFrag, PubChemLite for Exposomics, the PubChem PFAS Tree, patRoon, ShinyTPs and the Chemical Stripes.

How did you get involved in metabolomics?

Interestingly, through our need to fill the gaps in environmental resources via data sharing. Steffen Neumann (IPB Halle) was just setting up the first European MassBank server at the time – this was the conversation starter that spurred many joint activities (MassBank EU, MetFrag, CASMI) that have helped keep up my connections with the metabolomics community over the years. I'm honoured to have the opportunity to give a keynote at the 20th Metabolomics Society meeting in Osaka, Japan this year, which will be my first chance to visit the "home" of MassBank. I hope to see many of you there!

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

For me, it is the interdisciplinary bridging of the two (or more) worlds of environmental chemistry and systems biology – metabolomics vs exposomics – through informatics and now even through to digital history. It is interesting to learn and integrate new perspectives and find the common ground (or "trading zone" as our collaborator, C^{2}DH Director Andreas Fickers calls it). As a group, this involves exploring and understanding our environment (Aurich et al 2023, DOI: 10.1186/s12302-023-00805-5), identifying unknown metabolites with stable labeling (stay tuned!), and joining these two worlds (see next question) to even using music and visualizations to communicate the challenges we face processing millions of chemicals in our daily work!

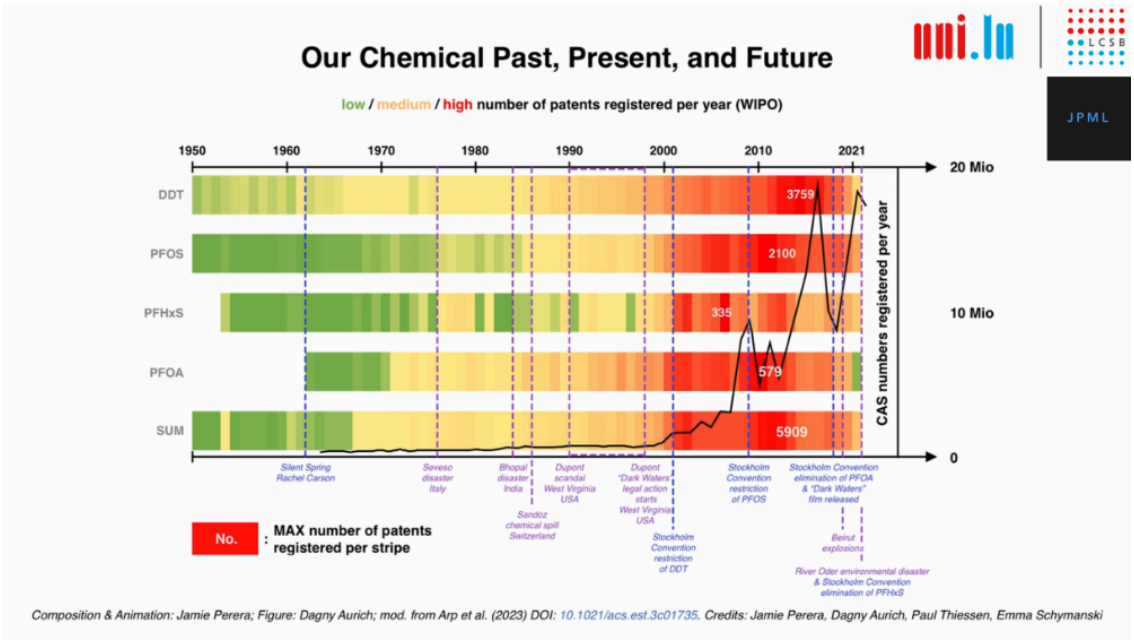


Figure 1: Our Chemical Past, Present, and Future. Composition and Animation: Jamie Perera. Figure: Dagny Aurich, modified from Arp et al., 2023, DOI: 10.1021/acs.est.3c01735. Credits: Jamie Perera, Dagny Aurich, Paul Thiessen, Emma Schymanski. Video on Vimeo, soundtrack on SoundCloud.

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

As a group, we contribute to a number of community developments, including MassBank Europe, the NORMAN Suspect List Exchange (NORMAN-SLE), MetFrag, PubChemLite for Exposomics, and the environmental non-target workflow patRoon (just to name a few). Our PhD students have started releasing packages of their own, including ShinyTPs by Emma Palm (DOI: 10.1021/acs.estlett.3c00537) to curate text-mined information and thus increase the amount of open transformation information available for approaches such as BioTransformer. Dagny Aurich has developed the Chemical Stripes package (see Figure 1) to explore patent information over time, which has made it really fun to explore the relevance of chemicals mentioned at environmental conferences. Beyond all these “tools” (hosted on infrastructure provided by our Bioinformatics Core), we collaborate closely with Carole Linster’s Enzymology and Metabolism group and the Systems Ecology group led by Paul Wilmes on the microbiome. Our internal collaborations with several other groups (Anne Grünewald, Jens Schwamborn, Michael Heneka) on exposomics are slowly coming to fruition, championed by Bego Talavera Andújar with her highly collaborative and integrative work on Parkinson’s DOI: 10.1007/s00216-022-04207-z) and Alzheimer’s (DOI: 10.1021/acs.est.3c10490) disease (see Figure 2) – this work has led to a lot of exciting new openings throughout LCSB, Luxembourg and beyond – stay tuned!

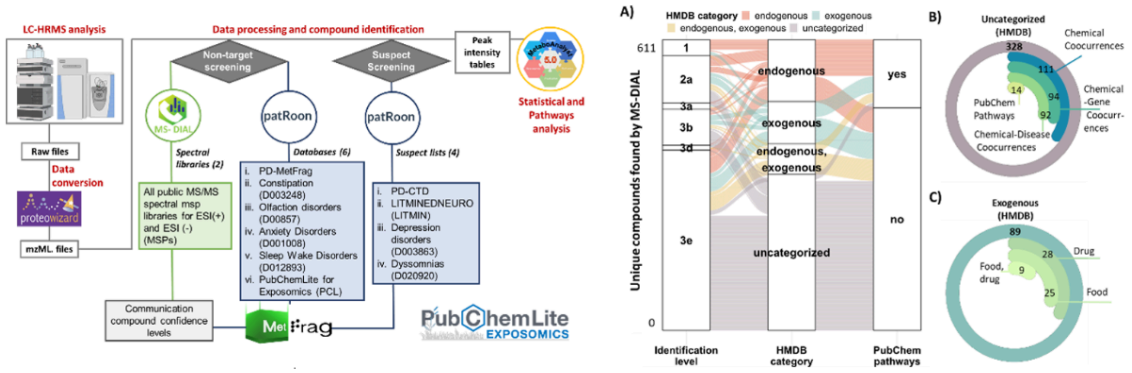


Figure 2: Exposomics workflows at ECI. Left: Exposomics (analytical and cheminformatics) data workflow for a Parkinson's disease case study, modified from Talavera Andújar et al., 2022, DOI: 10.1007/s00216-022-04207-z. Right: Exposomics in a Cerebrospinal Fluid Alzheimer's pilot study (A) Alluvial plot of MS-DIAL annotations, HMDB and PubChem annotation categories (B&C) Additional information available for the uncategorized and exogenous categories shown in A; images from Talavera Andújar et al., 2024, DOI: 10.1021/acs.est.3c10490.

What is happening in your country in terms of metabolomics?

For a small country, we have a relatively active biomedical focus (it is one of the research priorities of the country), so there is a lot of metabolomics going on at LCSB (where I am located) and the Faculty of Science, Technology and Medicine (FSTM), both at the University, plus activities at the Laboratoire National de Santé (LNS), Luxembourg Institute of Health (LIH) and even the Luxembourg Institute of Science and Technology (LIST). We also have an active network with our neighbouring countries, such as YoungNMC to support early career metabolomics researchers in the BeNeLux (Belgium, Netherlands, Luxembourg) region. One of the exciting new initiatives launching soon (pending final funding decision) is the Losch Centre for Rare Childhood Diseases coordinated by Carole Linster (LCSB) and Barbara Klink (LNS). This National Centre of Excellence in Rare Disease Research and Care will improve the health and quality of life of children suffering from a rare disease and their families in Luxembourg (and beyond) and will complement some of our newest projects, such as the European Joint Programme on Rare Diseases (EJP RD) consortium GENOMIT, with one of the largest rare mitochondrial disease cohorts available. We are looking forward to the opportunity to build on our joint work on the role of CLN3 in Batten's disease led by Ursula Heins-Marroquin et al (2024, DOI: 10.26508/lsa.202302057) and others.

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

We are lucky that our work seems to reach a wide audience given the size of our group (and country!). It is difficult to go to an environmental conference without hearing about the

“Schymanski levels” (more on this below) but we also see many users of patRoon, MetFrag, our NORMAN-SLE suspect lists, PubChemLite, etc. It is nice to see our contributions to MassBank EU emerge in MS-DIAL, MoNA, GNPS, and most recently PubChem (see Elapavalore et al., 2023, DOI: 10.1039/D3EM00181D). Through our various community efforts, it’s getting difficult to find a record in PubChem without some trace of us (somewhere!) – huge thanks and kudos to the entire PubChem team for supporting these community efforts! I also hope that we can continue to support new ideas and new ways of looking at things to the field, inspiring the next generation to do great things too. I would like to see a future where non-target exposomics is ready for routine use in solving problems – and would hope that we can contribute to this future.

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

The greatest strength of metabolomics, in my opinion, is you, the community. Together, the insights we all generate will help to build our understanding about metabolism and bring the whole field forward. This is not a scientific field that can thrive in a bubble, but our collective knowledge and understanding have the potential to have a great impact on many things.

What do you see as the greatest barriers for metabolomics?

The greatest barriers that I see are those that encourage competition over collaboration, profit over community, the constant need for “novelty” and “new” approaches rather than stabilizing and improving those that we have once they are “ready to go” (here I am especially referring to the community resources upon which many of us rely). Although machine learning and artificial intelligence (ML/AI) is all the rage right now, we still have too little (public) data, especially on the chemistry side, to truly profit from this yet. This especially applies to exposomics, where PubChemLite is ~380K molecules, PubChem itself 118 million chemicals … yet we only have toxicity data on a few thousand chemicals. Prioritizing these for realistic outcomes and actions is a really interesting challenge that we are currently trying to explore; see for instance our articles on “Per-and polyfluoroalkyl substances (PFAS) in PubChem: 7 million and growing” (DOI: 10.1021/acs.est.3c04855 or here: https://pubchem.ncbi.nlm.nih.gov/classification/#hid=120) and our preprint on substance grouping for persistent and mobile (PM) contaminants (Chirsir, Palm et al 2023, DOI: 10.26434/chemrxiv-2024-tn5t5) with our ZeroPM work package partners.

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

I had an interesting conversation the other day (thanks to Thomas Backhaus) that explored whether we need more and more new approaches – or rather to improve our knowledge base with what we already have. In many cases now for our efforts (see also above), experimental data is the limiting factor, yet there are few incentives to create and share this data (with the community). Of course, technologically and computationally many improvements could also be possible; but one issue we've also explored in our LuxTIME project is whether we (always) need the extremely resource-intense multi-omics approaches (of course necessary for deep biological understanding – yet many cohorts are only relatively recent) vs. e.g. delving into past literature to gain insights from "historical exposomics", including the grey literature (Aurich et al, 2023, DOI: 10.1093/exposome/osad007). There must be room for small players in this space, yet the expense of many investigations is putting "novel" efforts out of the reach of small research groups.

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

At the moment (and I noted that I was much more positive about this in the interview I gave 3 years ago) I would say it's patchy. It is getting harder and harder to get funding, especially for supporting computational infrastructure developments. Increasingly, this is going to the (very) big players in the field, yet even for some of them, it is getting harder to find infrastructure support to host resources upon which we all (and literally all of us) rely. I would wish for a more distributed system, where also the younger PIs have a chance to explore their ideas that may change the way we do things, as well as more general support for community infrastructure without having to constantly enclose these in "novel" questions. Many investigations are now extremely expensive; there must be space in the research environment for smaller initiatives too. Like many of my fellow researchers, I am becoming increasingly frustrated having to continuously apply for competitive funding with decreasing success rates (even projects highly recommended for funding are being rejected as the funding pool is too small) and seeing excellent colleagues really struggle to secure their future – in the end, there is no time left to do the research and a lot of energy is being wasted that could be better invested in our community efforts and the younger generation.

What role can metabolomics standards play?

This question is great timing! It is (coincidentally) the 10 year anniversary of the "Identification Level" scheme I proposed with Eawag colleagues for the environmental community in 2014 (Schymanski et al., 2014, DOI: 10.1021/es5002105), inspired partially by the Metabolomics Standard Initiative (MSI). None of us ever imagined at the time what an impact this paper would have. I am personally amazed at how this has endured and

how it still (and even increasingly) stimulates discussions today. Since our original publication, there have been many modifications and alternatives published; I am involved in some of them but certainly not all. Examples include our thoughts on integrating CCS with Celma et al., 2020, DOI: 10.1021/acs.est.0c05713, developing PFAS-specific levels with Charbonnet et al., 2022, DOI: 10.1021/acs.estlett.2c00206 and automating the assignment of confidence levels in patRoon (Helmus et al., 2021, DOI: 10.21105/joss.04029) and the NORMAN Digital Sample Freezing Platform (Alygizakis et al., 2023, DOI: 10.1016/j.trac.2023.116944). I know the metabolomics community is currently exploring a new system for their purposes, but this is proving challenging. Our levels deliberately focused on HRMS but extending this to identification in general in a manner that is applicable to all techniques is not a trivial exercise.

To get more technical, one standard I would definitely like to see adopted soon is our recent InChI proposal for specifying Isotopologue and Isotopomers (see preprint: Moseley et al. 2023, DOI: 10.21203/rs.3.rs-3727054/v1). I believe this proposal will be key for us to improve the annotation of metabolomics data for MS, NMR, and other techniques in a systematic manner compatible with current structural-based annotation, including accounting for uncertainties in the assignment of structural information based on available information.

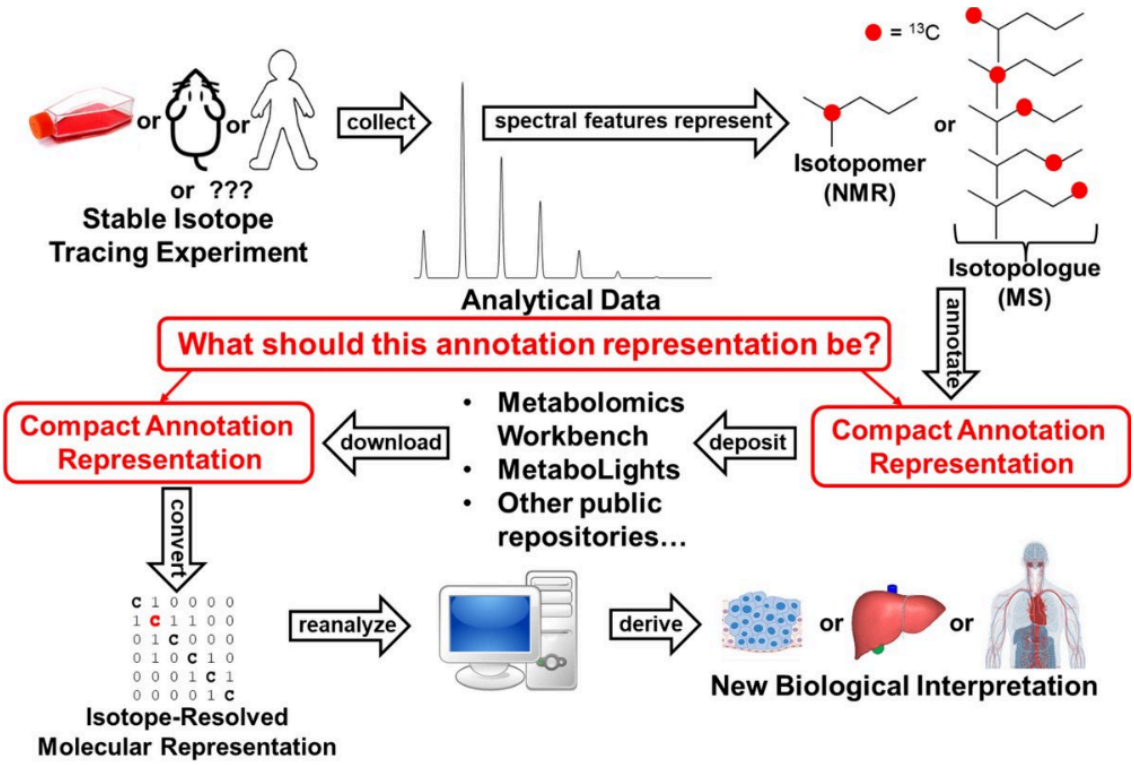


Figure 3: Overview of the isotopically resolved spectral feature annotation challenge. Source: Moseley et al. 2023, DOI: 10.21203/rs.3.rs-3727054/v1 (preprint).

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

The future is you, your ideas, enthusiasm, curiosity and insights (and the data that you share with the community) – I wish you all much success and enjoyment in exploring the wonderful world of metabolomics and exposomics!

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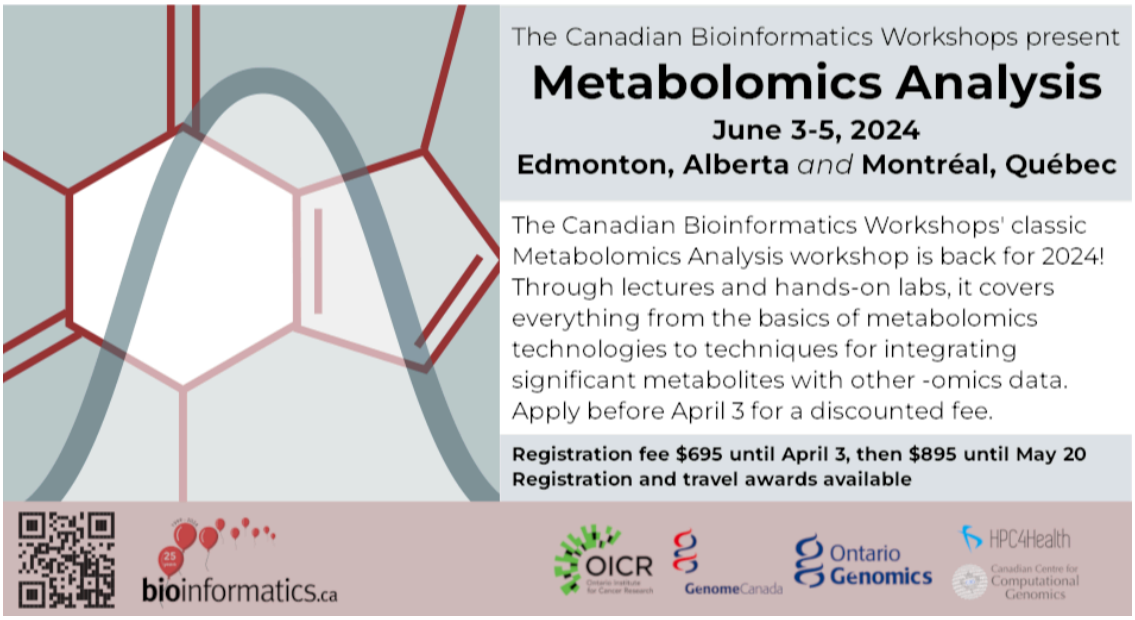

Recent Publications

Reviews:

- Advances in mass spectrometry-based multi-scale metabolomic methodologies and their applications in biological and clinical investigations (Open access)
- Metabolomic biomarkers for (R, S)-ketamine and (S)-ketamine in treatment-resistant depression and healthy controls: A systematic review
- Spatial analysis of the osteoarthritis microenvironment: techniques, insights, and applications (Open access)

Articles:

- An Integrated Metabolomics-Based Model, and Identification of Potential Biomarkers, of Perfluorooctane Sulfonic Acid Toxicity in Zebrafish Embryos

- Associations of multiple air pollutants with kidney function in normal-weight and obese adults and effect modification by free fatty acids
- Can Small Molecules Provide Clues on Disease Progression in Cerebrospinal Fluid from Mild Cognitive Impairment and Alzheimer's Disease Patients? (Open access)
- ChloroDBPFinder: Machine Learning-Guided Recognition of Chlorinated Disinfection Byproducts from Nontargeted LC-HRMS Analysis
- Early-life noise exposure causes cognitive impairment in a sex-dependent manner by disrupting homeostasis of the microbiota-gut-brain axis
- Effects of polystyrene, polyethylene, and polypropylene microplastics on the soil-rhizosphere-plant system: Phytotoxicity, enzyme activity, and microbial community
- Efficient Quantification of Milk Metabolites from 1H NMR Spectra Using the Signature Mapping (SigMa) Approach: Chemical Shift Library Development for Cows' Milk and Colostrum
- Environmentally Relevant Concentrations of Tetrabromobisphenol A Exposure Impends Neurovascular Formation through Perturbing Mitochondrial Metabolism in Zebrafish Embryos and Human Primary Endothelial Cells
- Flavor enhancement during the drying of scallop (Patinopecten yessoensis) as revealed by integrated metabolomic and lipidomic analysis
- Metabolic response of bacterial community to sodium hypochlorite and ammonia nitrogen affected the antibiotic resistance genes in pipelines biofilm
- Metabolomic profiles of sleep-disordered breathing are associated with hypertension and diabetes mellitus development (Open access)
- Metabolomics Provides Novel Insights into the Potential Toxicity Associated with Heated Tobacco Products, Electronic Cigarettes, and Tobacco Cigarettes on Human Bronchial Epithelial BEAS-2B Cells (Open access)
- Multi-omics reveal mechanisms of high enteral starch diet mediated colonic dysbiosis via microbiome-host interactions in young ruminant (Open access)
- Multiomics Analyses With Stool-Type Stratification in Patient Cohorts and Blautia Identification as a Potential Bacterial Modulator in Type 2 Diabetes Mellitus
- Programming a Ferroptosis-to-Apoptosis Transition Landscape Revealed Ferroptosis Biomarkers and Repressors for Cancer Therapy (Open access)
- Seasonal and daily patterns in known dissolved metabolites in the northwestern Sargasso Sea (Open access)
- Unraveling the potential of segment scan mass spectral acquisition for chemical isotope labeling LC-MS-based metabolome analysis: Performance assessment across different types of biological samples
- Untargeted 4D-metabolomics using Trapped Ion Mobility combined with LC-HRMS in extra virgin olive oil adulteration study with lower-quality olive oils

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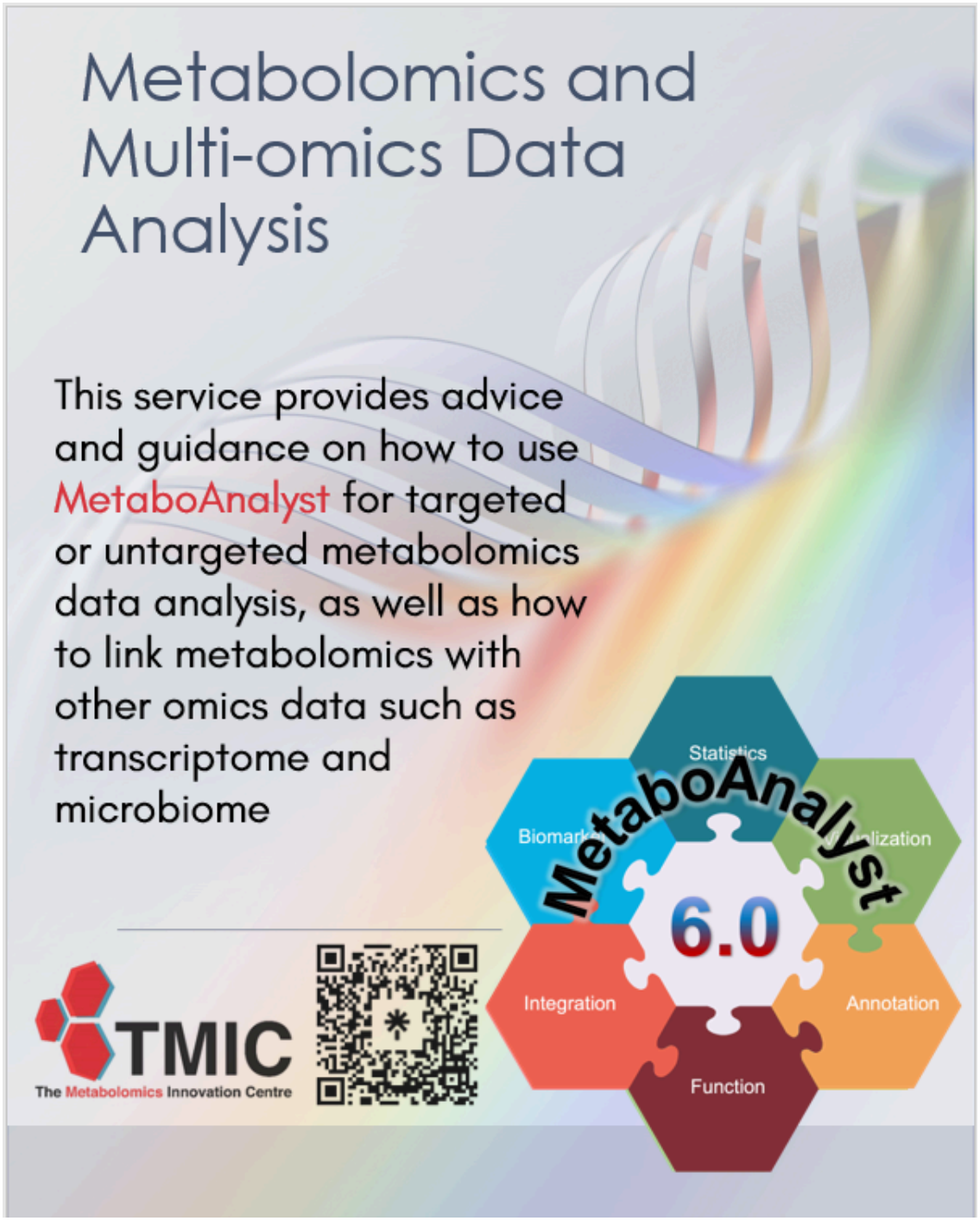

Metabolomics Events

MANA SODAMeet

April 9, 2024

Venue: Online

The goal of SODA is to provide a community-driven resource of actively-maintained software, test datasets used for software benchmarking, and results produced by software. SODAMeets is a platform where data generators and computational scientists can share their use of software/data. During SODAMeets (every 2 months), two speakers will present on software or data they would like to share with the community, emphasizing how these software/data are used. Speakers will be requested to fill out a form on our SODA website so that we collect relevant information on these software/data presented.

Join the web seminar

Bits & Bites # 03: Mass Spectrometry Imaging 101: Sample Preparation

April 11, 2024

Venue: Online

Bits & Bites 2024 is a flexible learning experience tailored for busy researchers seeking condensed yet impactful sessions. Now in its fourth year, this series continues to bridge the gap for those unable to commit to 1- or 2-week intensive courses.

10-part short course series will feature in-depth topics in untargeted metabolomics such as mass spectrometry applications, mass spectrometry imaging, statistics with both MetaboAnalyst and R, GNPS, MS-DIAL, and so many others. Each short course can be taken individually or you can select multiple Bites. Participants will gain a deeper insight into current software, methods, and

pitfalls. Each session starts promptly at 9 a.m. (Pacific Time) and will take approximately 4 hours. The courses will be conducted in a highly interactive manner, with the use of freely available software and databases. The tuition is $175 USD per Bite, except for #10. The tuition for #10 is $350 USD as it will take approximately 8 hours.

This 3rd course is led by Dr. Elizabeth Neumann from UC Davis, and offers an introductory look into the fundamentals of mass spectrometry imaging (MSI), with a focus on sample preparation techniques like tissue freezing, sectioning, and matrix application. Tailored for beginners with no required software or prerequisites, this short course aims to equip participants with essential skills in MSI instrumentation, data analysis, and visualization, providing a solid starting point for researchers and students embarking on MSI projects.

Check for more details

X-omics festival 2024

April 15, 2024

Venue: Nijmegen, Netherlands

The sixth edition of the X-omics festival “The future of multi-omics research is now!” will include:

- A keynote lecture
- Lectures from X-omics investigators on the X-omics facilities, innovative technologies, multi-omics data integration and multi-omics impact
- User pitches about innovative omics technologies
- A pitch your project session with the expert panel
- Scientific posters and poster pitches
- Networking opportunities

No registration needed. On the day of the event, it will be livestreamed via YouTube: X-omics festival 2024 - livestream.

Check for more details

Bits & Bites # 04: Quantification in Metabolomics: Tools for Robustness *New Course*

May 9, 2024

Venue: Online

The new course is taught by Dr. Huaxu Yu at UC Davis. This introductory course, requiring no specific software or prior knowledge, delves into the critical role of quantification in targeted metabolomics, essential for fields such as pharmacology and medicine. The course will cover fundamental quantitation principles, including selectivity, accuracy, and LOD/LOQ, and address common challenges like adducts and in-source fragmentation. Participants will also explore the distinctions between targeted and untargeted metabolomics, shedding light on essential concepts such as normalization techniques and what to consider when doing one or the other.

Check for more details

5th Annual Canadian Metabolomics Conference (CanMetCon) 2024

April 25 – 26, 2024

Venue: Vancouver, Canada

The 5th Annual Canadian Metabolomics Conference (CanMetCon) 2024 will be held in April 25-26, 2024 at the University of British Columbia, Vancouver, BC, Canada. This year, the conference presents an exciting two-day agenda: Day 1 is dedicated to "Metabolomics Technology and Integration", offering deep dives into the latest advancements and methodologies, while Day 2 focuses on "Multiomics and Applications". Registration for the conference is open, inviting researchers, students, and professionals to join this vibrant gathering of the metabolomics community!

Important dates:

- Last chance to register is until **March 22, 2024 (few tickets left only)**
- **Abstract Submission** Deadline: closed for Oral Presentation, **March 22, 2024** for Posters

Thanks to our generous sponsors, we are able to keep the Early-Bird registration fee rate at CAD 150 for students and CAD 250 plus applicable taxes and fees until March 22! Your registration fee includes a welcome reception on April 25, breakfast and lunch on April 25–26, and light refreshments during morning and afternoon coffee breaks.

Check out our updated conference program here.

Register now

5th EpiLipidNET Action Meeting

May 13 – 15, 2024

Venue: Dresden, Germany

EpiLipidNET is a pan-European network of scientists, clinicians, scientific societies, and enterprises aiming to create a hub of excellence with the focus on integrative lipidomics research. This network is funded by European Cooperation in Science and Technology and is an open community to all with an interest in (epi)lipids and related technologies. You can get more information about EpiLipidNET mission and achievements here.

5th Annual Meeting welcomec participants representing different fields of lipid research – from basic biochemistry and cell biology, to lipidomics technologies and clinical translation. Over three days, the program will include 7 scientific sessions with oral presentations, 2 dedicated poster sessions, and several social events to support networking and knowledge exchange.

Important dates:

- Registration deadline: **March 31, 2024**
- Abstract Submission Deadline: **March 31, 2024**

The preliminary program is here!

Register here

2024 Canadian Bioinformatics Workshop series: Metabolomics Analysis

June 3 – 5, 2024

Venue: Edmonton, AB and Montréal, QC, Canada

CBW's Metabolomics Analysis workshop taught by Dr. David Wishart and Dr. Jeff Xia is back in 2024! Through lectures and hands-on labs, this three-day course will teach participants to:

- Design appropriate metabolome-focused experiments
- Understand the advantages and limitations of metabolomic data analysis
- Devise an appropriate bioinformatics workflow for processing and analyzing metabolomic data
- Apply appropriate statistics to undertake rigorous data analysis
- Visualize datasets to gain intuitive insights into the composition and/or activity of their metabolome
- Integrate metabolomics data with SNPs, transcriptomics, and microbiome data

Applicants can choose to attend in either Edmonton or Montréal. Apply before April 3 for a discounted registration fee.

More information here: bioinformatics.ca
When: June 3-5, 2024
Where: Edmonton, Alberta and Montréal, Québec
Cost and deadlines: $695+GST before April 3, then $895+GST until May 20

Register for Workshop

Imperial College London Metabolomics training course: Hands-on Data Analysis for Metabolic Profiling

June 10 – 14, 2024

Venue: in-person at London Hammersmith campus, UK

This 5-day course provides a comprehensive overview of data analysis for metabolic profiling studies focusing 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.

Registration is open and will close on **May 29, 2024.**

MRC-funded bursaries are available to cover the full early bird fee. The deadline for applying for a Bursary is 19 April (12.00 BST).

Learn more about the course

20th Annual Conference of the Metabolomics Society Metabolomics 2024

June 16 – 20, 2024

Venue: Osaka, Japan

20th Annual International Metabolomics Conference of the Metabolomics Society will be held on June 16-20, 2024 in Osaka, Japan. The conference is the official annual meeting of the Metabolomics Society, and the largest metabolomics meeting worldwide. Save the upcoming dates:

- Oral Abstract deadline: Closed on March 14, 2024 (extended from March 7)
- Poster Abstract deadline: **May 16, 2024**

Scientists in academia, government, industry, and others working in the field of metabolomics are invited to submit abstracts in the following scientific themes:

- Metabolomics in Human Health and Disease
- Plants, Food, Environment and Microbes
- Technology Advancements
- Computational Metabolomics, Statistics & Bioinformatics
- Industry Spotlight: Metabolomics in Pharma and Biotech

Learn more here

16th Mass Spectrometry School in Biotechnology and Medicine

July 7 – 13, 2024

Venue: Dubrovnik, Croatia

The MSBM program is taught through a combination of lectures, workshops and tutorials. It is suitable for attendees from a wide variety of backgrounds, and the standard core syllabus covered every year is as follows:

- Mass spectrometry basics
- Introductions to main classes of mass analysers – ToF, ion traps, quadrupoles, FTMS etc.
- Ionization sources – ESI, MALDI etc.
- Ion mobility
- Separations methods – LC, CE, HILIC, fractionation etc.
- Tandem MS – CID, ECD, UVPD, SRM, MSM, DDA, DIA etc.
- Mass spectrometry systems – e.g. LC-ESI-QToF, IMS-MSMS etc.
- Proteomics – bottom-up, top-down, quantitative etc.
- Other omics – lipidomics, metabolomics, glyomics etc.
- MS data processing and Informatics

Registration is open now and will close on **June 12, 2024.**
For more information, please visit msbm.org or send an email to msbm.dubrovnik@gmail.com

Learn more here

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NIST SRM 1950 Beyond the Certificate of Analysis: mQACC Call to Provide Qualitative and Quantitative Data

Certified reference materials (CRM) values provide a known and standardized reference point against which the results of a metabolomic study can be compared. However, the certification of hundreds of individual metabolites is a cumbersome and time-consuming process. The Standard Reference Material (SRM) 1950, Metabolites in Frozen Human Plasma, is by far the most used reference material by the metabolomics community. NIST SRM 1950 provides certified and/or reference values for select metabolites and lipids such as fatty acids, electrolytes, vitamins, hormones, and amino acids. The metabolomics community would greatly benefit from consensus values and identification of metabolites and lipids in SRM 1950 that are not tied to a single analytical platform or method. This increases the accuracy, reliability, harmonization, and meaningful comparisons of metabolomic studies utilizing the material. Additionally, having more values and information available for SRM 1950 metabolites and lipids would allow researchers to investigate a broader range of analytes in their studies, which in turn could lead to a better understanding of the underlying biology of the metabolic processes. To that end, the Reference and Test Materials Working Group of mQACC is actively collecting information on qualitative identifications and quantitative values of metabolites and lipids in NIST SRM 1950 beyond those listed on the NIST Certificate of Analysis. Any data from instrumental platforms with compound identification (LC-MS, GC-MS, NMR) are welcome to participate. The data was combined in order to produce a publicly available database of community-generated 1) consensus concentration values for quantified metabolites and lipids of critical interest within the community and 2) compounds identified but not quantified in SRM 1950.

More information and an example reporting form can be found at https://www.mqacc.org/srm1950

Metabolomics Jobs

Metabolomics Jobs

If you have a job to post, please email the MetaboNews team at metabolomics.innovation@gmail.com

We may remove a listing after 6 months if we do not receive a confirmation that it is still necessary. However, if you would like us to repost it, please contact us.

Job Title	Employer	Location	Source
Post Doctoral Position in Human Nutrition: Metabolomics-based exploration	The French National Research Institute for Agriculture, Food, and the Environment (INRAE)	France	INRAE
Post Doctoral Fellow in Metabolomics	Michigan State University	East Lansing, MI, USA	Michigan State University
Assistant Professor, Applied Metabolomics	The Ohio State University	Columbus, OH, USA	The Ohio State University
Postdoctoral Fellow – Microsampling devices for lipidomics	Concordia University	Montreal, QC, Canada	The Metabolomics Innovation Centre (TMIC)
Postdoctoral Research Associate in Metastasis Metabolism	Nuffield Department of Surgical Sciences , University of Oxford	Oxford, UK	Metabolomics Society
Canada Research Chair (CRC) Tier 2 in Metabolomics	Schulich School of Medicine and Dentistry, Western University	London, ON, Canada	Western University
Chemical Biologist/Ecologist	The Monell Chemical Senses Center	Philadelphia, PA, USA	The Monell Chemical Senses Center
ORISE Postdoctoral Fellowship in Pharmacology/Toxicology	National Center for Toxicological Research U.S. Food and Drug Administration	Jefferson, AR, USA	Metabolomics Society
ORISE Postdoctoral Fellowship in Neuroscience/ Neurotoxicology	National Center for Toxicological Research U.S. Food and Drug Administration	Jefferson, AR, USA	Metabolomics Society

MetaboNews Feedback Form

Thank you for being a part of MetaboNews! Your input means a lot to us, and we're eager to hear your thoughts on how we can improve our newsletter. We've put together a brief, anonymous survey with just two mandatory questions that won't take more than a minute of your time. Your feedback is invaluable, so please take a moment to share your opinions with us.

Fill Out Your Survey Here

If you have any questions, don't hesitate to contact us at metabolomics.innovation@gmail.com

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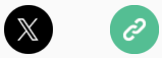

Our mailing address is:
metabolomics.innovation@gmail.com