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MetaboNews

This month in metabolomics

December, 2024
Vol 15, Issue 1

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

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Perspectives
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Towards Single Cell Metabolomics

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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

The Metabolomics Society along with the Scientific Organizing Committee are delighted to extend this invitation to you to attend Metabolomics 2025, the 21st Annual Conference of the Metabolomics Society, in Prague, Czech Republic. The conference will be held June 22-26, 2025 at the Prague Congress Centre.

Metabolomics 2025

Prague Congress Centre
June 22 - 26
www.metabolomics2025.org

The website will be continually updated, check back often for updates.
Follow **@MetabolomicsSoc** on X to stay current and meet new peers before the event!

Abstract Submission
Abstract submission is now open, with a deadline of **March 6 for oral abstracts** and May 15 for poster abstracts.

You can apply for one of the numerous travel awards offered by the Society and affiliates when you submit your abstract. Review all requirements on the **awards page**.

Conference registration will be available in the next couple of weeks. Stay tuned for announcements.

Calling all Sponsors!
The **Sponsorship Brochure** is available online, we still have a few opportunities available!

As we approach the conference, we look forward to partnering with your organization to continue the success of bringing together all the major international organizations involved in human, plant, microbial, animal, and environmental metabolomics.

We have a variety of packages available to position your brand and product at the forefront of the scientific community. Your support is extremely important to the success of the meeting, helping to keep registration costs down, which allows more of our younger scientists to attend. We look forward to partnering with you for Metabolomics 2025!

Members' Corner

Board of Directors

Dear Metabolomics Society Members and metabolomics friends,

Welcome to 2025 and I hope all enjoyed some rest and relaxation during late December. We are only a few weeks into 2025, but the Board of Directors have been working hard on many aspects of the Societies operations.

Natasa and Tomáš along with the scientific organising committee (SOC) are working hard on developing the programme for Metabolomics 2025 to be held in Prague. They have received an avalanche of high-quality workshop proposals, too many to be able to host all the proposed workshops, so thank you to all who submitted a proposal. If you are not successful this year do consider applying again in future years. The abstract submission portal is currently open, please do consider submitting abstracts for oral presentations or posters. Importantly, the SOC hope to see many applications from scientists early in their career. All abstracts are reviewed by multiple members of the SOC and all abstracts are blinded (i.e. the reviewers do not see the authors or affiliations information).

Roy along with Matej and Maria have been working hard on a new mechanism to support the metabolomics community. An ECR mobility award has been developed to help financially support Early Career Researchers and Technical Experts who are members of the *Metabolomics Society* to go to a Host Institution for a short period (two weeks minimum to three months maximum) to learn something new in the area of metabolomics (and related sciences such as lipidomics) and to then bring this knowledge and know-how back to their own Home Institution. The maximum award will be for $2500. This will be announced in more detail soon.
Other exciting topics and developments will be communicated during the next 12 months.

Finally, I hope to see some of you at the GRC Metabolomics 2025 conference in Ventura, California in early February (and do come and say hi!). At the date of writing, the conference is still to be operated, and all attendees will be updated nearer the conference. Our thoughts go out to all affected by the tragic events we are observing in Los Angeles. I have had the pleasure to work with Susan Sumner to chair the conference and we look forward to great scientific discussions.

All the very best,

Warwick (Rick) Dunn, University of Liverpool, UK
President, Metabolomics Society

The 6th Annual Canadian Metabolomics Conference is taking place in Montreal, Canada from April 24-25th. This event will bring together top researchers, professionals, and students from across the metabolomics field for two days of discussions, presentations, and networking opportunities.

The conference will feature plenary and keynote lectures from prominent experts in the field, including:

- **Dr. Erin Baker** (University of North Carolina) – *"Exploring Lipidomic Perturbations Due to Chemical Exposures"*
- **Dr. Mary-Ellen Harper** (University of Ottawa) - "*"Leveraging*

metabolomics and systems biology approaches in the clinical translation of cellular bioenergetics research”"

- **Dr. Gary Siuzdak** (Scripps Research) – *“Sifting through Analytical Artifacts: Untargeted Activity Metabolomics and Data Mining Yield Gold”*

Additional keynote presentations will include contributions from leading researchers such as Dr. Lorraine Brennan, Dr. Matej Oresic, and Dr. Tom Metz, and many others, covering a range of topics from Clinical Metabolomics, Computational Metabolomics and Machine Learning, Metabolomics of Nutrition and Health, and Public Health and Population Metabolomics.

Follow the link for registration details: Registration Link

Early-Career Members Network (EMN)

EMN Webinars 2024-2025

January Webinar

The first webinar of the new year was hosted by **Prof. Dr. Wout Bittremieux**, assistant professor in the Adrem Data Lab at the University of Antwerp, Belgium titled: “*Learning From Repository-Scale Untargeted Metabolomics Data*”. The recording will soon be posted on MetSoc website and YT channel. We thank Prof. Bitremieux for his time and exciting webinar!

February Webinar

The second EMN webinar will take place on Wednesday, 12th February 2025, at 15:00 UTC (16:00 CET), featuring **Prof. Dr. Judith Jans** and **PhD candidate Hannah German** from UMC Utrecht, Netherlands. The EMN committee is delighted to invite you to a talk on "*Applications of metabolic flux analysis in the field of inborn errors of metabolism*", focusing on clinical metabolomics. The registration link will be available soon.

Online Presence

Keep an eye on your inbox for email blasts and make sure to follow us on our social media accounts: Twitter, Bluesky, and LinkedIn! This year, we especially encourage researchers from South America, Africa and Asia to participate in our webinars. If you are interested, or want to recommend someone from your network, please reach out to us at info.emn@metabolomicssociety.org.

ECR Voices

The EMN “ECR Voices” initiative to spotlight early-career researchers (PhD students,

Postdocs, Young Investigators, etc.) on our Twitter/X account is continuing through 2024-2025! You can check out an example here: (https://x.com/EMN_MetSoc/status/1704787637591265456?s=20). We encourage everyone to participate! You can easily create your own ECR Voice slide using this link: (https://docs.google.com/presentation/d/1H43FIlp3gmtJMUYS6r-2XVd460N8PjBn/edit#slide=id.p15).

The link contains instructions, templates, and examples from other researchers already featured on our Twitter/X page. It's as simple as making a single PowerPoint slide with a headshot and a few bullet points about yourself! Please consider sharing ECR voices with your network! This year, we would like to invite the researchers especially from South America, Africa and Asia to participate. If you are interested, or want to recommend someone from your network, please reach out to info.emn@metabolomicssociety.org.

Task Groups Corner

International Affiliations Task Group

Next meeting of the international affiliates will be on March 4, 2025 (online), followed by in-person meeting during the Metabolomics 2025 conference in Prague.

The affiliates training network is starting to take shape. A **template** was developed (by one of the affiliates, RFMF) for each affiliate to fill in information about the group/laboratories willing and able to participate in the training network.

International Affiliates' Corner

Australia & New Zealand Metabolomics Society (ANZMetSoc)
Visit https://anzmetabolomics.org/what-we-do

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Join us for AUS-oMicS 2025 in the heart of sub-tropical Cairns, a charming city with breathtaking views and abundant native wildlife in Queensland, Australia. This premier event incorporates the Australasian Proteomics Society, Australian and New Zealand Metabolomics Society, Australian and New Zealand Society for Mass Spectrometry and Australian Glycoscience Society, bringing together the leading minds in the field.

Whether you're an academic, industrial researcher, young scientist, or student, AUS-oMicS 2025 offers unparalleled opportunities for engagement, networking, and peer-to-peer learning. Discover new solutions, motivations, perspectives, and possibilities while enjoying the natural beauty of Cairns.

Visit us at: https://www.ausomics.com/

The deadline for oral abstract submissions and early bird registrations is fast approaching. Take advantage of this opportunity to showcase your work and secure your spot!

Oral abstracts: Submit by January 31, 2025
Poster abstracts: Submit by March 14, 2025
Submit your abstracts today: ausomics.com/abstracts

ANZMetSoc is supporting students and early career researchers with **travel awards** of up to $500 AUD to attend AUS-oMicS 2025. Applications will open soon—stay tuned for updates: anzmetabolomics.org

Réseau Français de Métabolomique et Fluxomique (RFMF)

Visit http://www.rfmf.fr/

Renewal of RFMF Junior Board

Each year, half of the RFMF Junior Board is renewed. At the beginning of 2025, 5 members were elected, 3 of them for the first time. We are pleased to present Nathalie LACRAMPE, operational coordinator and technical manager of the P2M2 facility in Rennes, Anouar MEJAIT, a recent PhD graduate working on the degradation of biopesticides and their impact on biodiversity at the CRIOBE laboratory in Perpignan, and Jeremy MONTEIRO, a recent PhD graduate who used metabolomics and lipidomics approaches to characterise dried blood spots. We are also pleased to announce that for this year, the junior board is led by Marine LETERTRE (president), lecturer at the University of Nantes and researcher at the CEISAM laboratory, Chloé CLOTEAU (vice-president), postdoctoral researcher at the M-shark platform in Nantes, Amandine ROCHER (treasurer), engineer at the MetaToul-MetaboHUB facility in Toulouse, and Thomas BRUNET (communications manager), clinical research project manager at HCL in Lyon. To find out more about our entire Junior Board of Directors, we invite you to visit our website at https://www.rfmf.fr/ca-junior-2025/.

RFMF Board of Directors Meeting in Nantes

The RFMF Board of Directors met in Nantes on 9 and 10 January, bringing together the senior and junior boards. It was an opportunity to get together physically and review current and future actions. A number of exciting initiatives should be launched in 2025 to promote access to and training in metabolomics and fluxomics. All in good science and good food ;)

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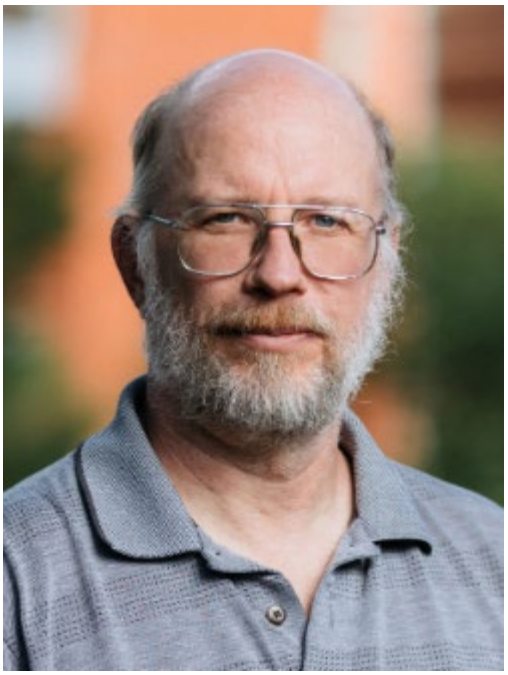
Perspectives

In our new *Perspectives* section, we take some time to sit down with experienced and decorated researchers in the field of metabolomics to gain their insights on both the evolution of the field and its future directions.

For our first *Perspectives*, we're excited to feature Dr. David Wishart, a leading figure in metabolomics, who shares his views on where the field has come from and where it's headed.



Dr. David Wishart (PhD Yale, 1991) is a Professor in the Departments of Biological Sciences and Computing Science at the University of Alberta. He is the founder and Co-Director of The Metabolomics Innovation Centre

From your perspective, when did metabolomics begin to gain prominence in the broader 'omics' world?

I think metabolomics really started to gain prominence in 2007/2008 with the International Metabolomics Society conferences in Manchester (2007) and Boston (2008). These conferences, which were very well attended, really helped to put the field of metabolomics "on the map". Both conferences raised the profile of metabolomics amongst other 'omics researchers as well as many established biomedical scientists. They also led to new funding initiatives in the US, Europe, Canada and Australia that helped give metabolomics a firmer foothold. The other catalytic event was the appearance of the Human Metabolome Database (HMDB) in 2007. We developed the HMDB through the support of a Genome Canada grant called the Human Metabolome Project (HMP). I believe the release of the HMDB made metabolomics much more accessible to aspiring metabolomics scientists. The HMDB did this by providing freely available reference information about metabolites (metabolite structures, nomenclature, descriptions, pathways, spectra) to the entire metabolomics community. In effect, the HMDB became the metabolomics world's equivalent to GenBank (for genomics) and UniProt (for proteomics). Over time, the HMDB has evolved to more fully connect the metabolome with the proteome and the genome. This multi-omics connectivity within the HMDB has also helped make metabolomics more visible to the broader 'omics world.

Reflecting on your journey, what is the most valuable piece of advice you would give to a new researcher entering the field of metabolomics?

I guess the short answer is: “Be nimble”. Science is evolving quickly, far more quickly than it did 50 years ago, 20 years ago or even 10 years ago. In the “old days” it was pretty common for scientists to train and specialize in an area of science and expect to have a long career doing mostly the same thing. These days you can’t expect to pursue the same scientific goal or use the same technology for your entire scientific career.

In my own case, I’ve changed “careers” at least five times. I started off as a structural biologist and my technology focus was NMR. Later on, I switched to pharmaceutical chemistry and my technology focus was peptide synthesis. Then I moved to bioinformatics and my technology focus was computers. Subsequently, I switched to metabolomics and my technology focus became mass spectrometry. More recently I’ve jumped into computational chemistry and my technology focus has become machine learning. At the same time, I’ve had to diversify my skillset beyond science to learn how to launch, finance and run small companies, to manage core facilities, to teach and organize workshops and to set up various engineering and electronics labs. Each of these changes has been a bit scary and often rather disruptive, but I’ve learned a lot and more importantly, I’ve learned how to be nimble, flexible and open minded. I’ve also realized that science is a lifelong journey of learning.

What are the largest barriers currently facing metabolomics? Are there limitations to how metabolomics can be implemented in research?

Metabolomics is facing some of the same challenges that historically stifled proteomics and transcriptomics – namely: 1) lack of reproducibility and 2) lack of coverage. I believe the issue of reproducibility is perhaps the most important. It seems to arise from our almost single-minded focus on metabolite identification instead of metabolite quantification. Quantification is key making metabolomics more reproducible. It is also key to moving metabolomics out from the research lab and into practice. If you want to use metabolomics in the clinic, you have to report accurate metabolite concentrations. If you want to use metabolomics in environmental monitoring, you have to report accurate chemical concentrations. If you want to use metabolomics in forensic science, agriculture, aquaculture, forestry or any other application, you have report accurate compound concentrations. Likewise, if you want to standardize metabolomics, share metabolomics data with other labs, or make metabolomics methods more reproducible, you need to focus on metabolite quantification. In other words, my main message is “quantify, quantify,

quantify".

Obviously, incomplete metabolite coverage is another challenge facing metabolomics. Most other fields of omics science achieve near complete genome, transcriptome or proteome coverage, but metabolomics is typically only able to cover 5-10% of the known or detectable metabolome. Incomplete spectral reference libraries, incomplete chemical libraries and limitations with instrument sensitivity are all contributing to this problem. However, I don't think that this lack of metabolite coverage is as serious as many believe. Our own experience, and that of many others, is that Nature tends to re-use the same modest number (500-600) of metabolites for responding to very different physiological stressors or insults. While I do expect that complete or near-complete metabolome coverage will soon be possible, I don't view it as much as a threat or challenge to metabolomics as the lack of reproducibility (i.e. the lack of quantification).

What role do you see for artificial intelligence and machine learning in metabolomics research and applications?

Artificial intelligence (AI) and machine learning (ML) are going to radically change how we do science, and certainly how we do metabolomics. Obviously, ML is already widely used in metabolomic data analysis. For instance, everyone uses PLS-DA or OPLS-DA or logistic regression, although they may not know these are ML techniques. However, ML is now being used to help identify novel metabolites (SIRIUS, MSNovelist, DeepMet), to predict MS/MS spectra (CFM-ID, FraGNNet), EI-MS spectra (NEIMS) and NMR spectra (PROSPRE and CASPRE). ML can also be used to accurately predict retention times for almost any chromatographic condition (RTPred) and retention indices (RIPred). The ability to accurately predict spectra and/or retention times opens the door to creating vast libraries of predicted spectra and corresponding RT/RI pairs, which will make compound identification much easier and faster. Likewise, new ML methods are being used to predict novel metabolite structures (DarkNPS and other chemical language models), metabolic transformations (CypReact, BioTransformer) and metabolic-fate pathways (BioTransformer). Over time, these tools will undoubtedly get better, faster and more accurate. I foresee a time in the not-to-distant future where these ML methods will allow 80-90% of all detected signals in MS/MS or EI-MS spectra to be confidently identified. In other words, I predict that AI and ML will largely solve the metabolite coverage problem. Other areas where ML is going to make a difference will be in helping to interpret metabolomics data. Large language models (LLMs), in particular, are going to greatly extend what is contained in metabolite and pathway databases. LLMs will also fundamentally change how we query or interact with these databases. LLMs will soon be able to act as intelligent metabolomics assistants, helping us write code, perform

workflows, integrate multi-omic information or intelligently interpret our data. Likewise, ML will also make data processing (peak picking, peak integration, peak comparison) faster, more accurate and more reproducible. Overall, I expect the benefits of AI and ML will be enormous and will make metabolomics even better, faster and cheaper than it is now.

Where do you see metabolomics in 10 years?

I think metabolomics will be very different than what it is now. First, I expect that the issue of limited metabolite coverage will be largely solved and that it will be very routine to accurately identify and even quantify 10,000+ metabolites in a single LC-MS run. Second, I expect metabolomics will be almost completely automated or roboticized and, hopefully, far more standardized. This will be done through a combination of cheap robots (perhaps made via modified 3D printers), low-cost fluidics or chip systems and AI. That means that metabolomics will be much more reproducible as well as much faster, less costly and far easier to do. Thirdly, I expect that metabolomics will be more frequently done using inexpensive, portable, handheld systems, rather than using big, expensive MS or NMR systems. The use of portable near or mid-infrared (NIR or MIR), portable Raman, portable colorimetric, portable electrochemical, portable ion mobility spectrometry (IMS) systems, benchtop NMR – or combinations of each, will be much more widespread. This is because AI and ML will allow more precise interpretation of these normally hard-to-interpret spectral measurements. These spectral interpretations will be aided by data originally collected by high-end NMR or MS, but the NMR and MS data will simply be used as training data for these portable systems. This shift should allow metabolomics to become more widespread in clinical, environmental, agricultural or at-home testing. Fourth, I expect that metabolomics, as a stand-alone research enterprise, will mostly disappear. It will be replaced by multi-omics or system-wide studies where combinations of quantitative metabolomics, proteomics, genomics and transcriptomics measurements will be the norm. This is simply a natural progression for any scientific field, especially as it matures and becomes more routine or more applied. Finally, and especially outside of the research lab, I expect metabolomics will become an integral part of everyday life, being used in many areas of medicine, agriculture and environmental work, enabling the widespread implementation of precision nutrition, precision medicine and precision agriculture. In other words, I see metabolomics as (finally) making a positive difference in not only our health, but the planet's health too.

What actions do you think are crucial for further growing the metabolomics field?

Metabolomics has always been viewed as the “poor cousin” of genomics or proteomics. That’s because it was technically the last field of omics science to emerge in the 1990s. As a result, it never got the massive financial support ($billions) or high-profile press coverage that genomics or proteomics received. Metabolomics scientists also don’t do a very good job of selling their science or trumpeting their successes. So, based on these observations, I think some of the actions that are needed to grow metabolomics are: 1) highlighting the importance of metabolomics and exposomics to human and planetary health; 2) trumpeting the successes of metabolomics to the media, to funders, to clinicians and to the public; 3) exploiting the strengths of metabolomics (fast, comprehensive, inexpensive, quantitative chemical measurements) to create more real-world, everyday applications.

In terms of action item #1, we need to constantly remind anyone who will listen that 95% of the causes of death are not genetic, but environmental (i.e., the exposome). This fact is not widely known, but it is being affirmed over and over in epidemiological studies. This means that focusing on the genome is the wrong thing to do and focusing on the exposome/metabolome is the right thing to do. In terms of action item #2, we need to remind people, especially funders and clinicians, that unlike genomics or proteomics, metabolomics has already been widely adopted by clinicians (most of whom don’t know it) and that it is poised to be even more widely used in the clinic. Metabolomics tests (i.e., newborn screening) are the most widespread and most impactful omics testing services ever offered. Almost everyone in the developed world, under the age of 35, has had a metabolomics test and these tests and the actionable interventions that come from them have saved more than 1 million lives. This level of impact is many times greater than the clinical impact of genomics testing. In terms of action item #3, the metabolomics community must focus on translational research. Rather than focusing on the how’s and why’s of metabolism, metabolomics must focus on questions such as “how can metabolomics be used to solve a common problem?” or “how can metabolomics be used more widely?” or “how can I convince a clinician to use my assay?”.

TMIC Wishart Node at The 5th Annual Canadian Metabolomics Conference

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Spotlight Article

Towards Single-Cell Metabolomics

Why Small Samples?

Traditionally, metabolomics assays are applied to collected biofluids, like a blood or urine sample, allowing for a metabolic snapshot of a whole organism. However, in many cases, collecting a sample from a whole organism is impractical. Now, these ‘small’ samples can now benefit from the power of metabolomics - accelerating a drug development pipeline, improving the sensitivity and accuracy of an in-vitro study, or revealing new insights into a cell culture model.

Analyzing Small Samples With Precision

TMIC’s Li Node offers the SHARP Metabolomics Cell Assay, a small-scale, highly accurate and reproducible platform for cell metabolome analysis providing maximum insights with minimal cells.

The SHARP (Small-Scale Highly Accurate and Reproducible Platform) Metabolomics Cell Assay provides an advanced service that empowers researchers working with minimal cell samples by delivering high-sensitivity metabolome profiling through advanced liquid chromatography-mass spectrometry (LC-MS). This platform brings the enhanced peak pair detection and high-confidence metabolite identification of TMIC's CIL-LC-MS assay to smaller applications - tissue culture models in drug development, in vitro biomarker discovery, and cellular biology, letting researchers assess the metabolome of as few as 5,000 cells at a time!

Key Features of SHARP Metabolomics Cell Assay

- Low Cell Numbers: Advanced Chemical Isotope Labeling LC-MS technology designed to analyze samples with as few as 5,000 cells. Ideal for working with scarce or valuable cell materials.
- Comprehensive Metabolome Coverage: Optimized separation and ionization enhance metabolite detection and high-confidence metabolite identification.
- High Accuracy and Precision: Unique "one to one" internal standard approach enables superior quantification.
- Cutting-Edge Instrumentation: Powered by the Thermo Scientific Vanquish NEO LC system integrated with the Orbitrap Exploris 240 Mass Spectrometer.

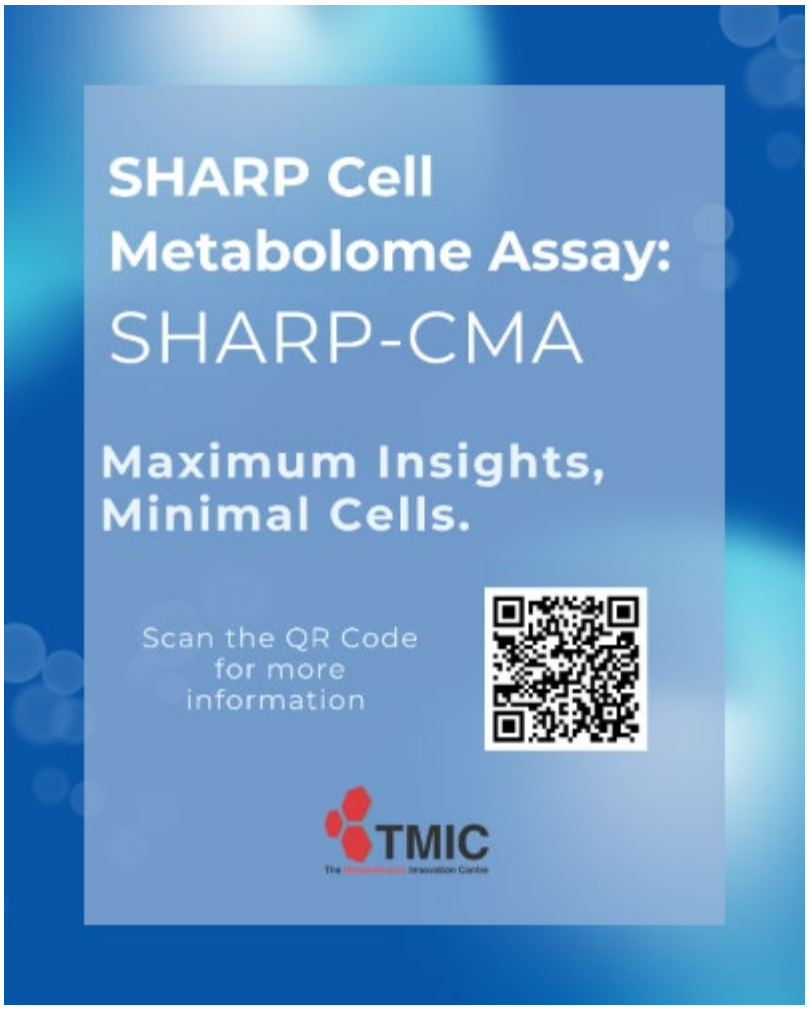
Tailored Service Options to Meet Your Needs

- Basic SHARP Cell Assay: Targets amine/phenol-containing metabolites, including amino acids, dipeptides, polyamines, and more.
- Elevated SHARP Cell Assay: Expands coverage to include amine-, phenol-, and carboxyl-containing metabolites, such as amino acids, dipeptides, short-chain fatty acids (SCFAs), and TCA cycle intermediates.
- Comprehensive SHARP Cell Assay: Provides the most extensive coverage, encompassing all metabolites included in the Basic and Elevated assays, along with hydroxyl- and carbonyl-containing metabolites.
- Flexible SHARP Cell Assay: Offers customizable options to focus on specific metabolite types based on your research needs.

Get Started Today

Unlock the power of metabolomics for your small sample research with the SHARP Metabolomics Cell Assay. Whether you ae developing new therapeutics, discovering biomarkers, or exploring cellular biology, our assay provides the sensitivity, precision, and flexibility you need.

For more information click here or contact us today at info@metabolomicscentre.ca



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MetaboReads

Immunomodulation and Inflammatory Disorders

These studies underscore the power of metabolomic analyses in revealing how immune cell activity and inflammation can be modulated. From identifying key metabolites such as lactate and bile acids to characterizing short-chain fatty acids, researchers are decoding the metabolic underpinnings of immunological balance. By mapping these shifts, novel interventions become possible, targeting precise molecular pathways to reduce tissue damage and restore immune homeostasis.

Multiomics analyses reveal adipose-derived stem cells inhibit the inflammatory response of M1-like macrophages through secreting lactate

Horie and colleagues in STEM CELL RESEARCH & THERAPY showed that adipose-derived stem cells (ADSCs) secrete lactate, which suppresses the inflammatory response in M1-like macrophages. They used targeted metabolomics to find high lactate concentrations in ADSC-conditioned medium and demonstrated that lactate significantly reduced the expression of pro-inflammatory genes. Interestingly, lactate did not cause M1-to-M2 macrophage polarization but instead epigenetically altered macrophages by inducing H3K27 acetylation. Pharmacological blockage of lactate uptake reversed ADSC-mediated anti-inflammatory effects, confirming lactate's central immunomodulatory role.

Lactobacillus acidophilus ameliorates cholestatic liver injury through inhibiting bile acid synthesis and promoting bile acid excretion

Wu and colleagues in GUT MICROBES found that Lactobacillus acidophilus ameliorates cholestatic liver injury by restraining bile acid synthesis and promoting bile acid excretion. Using a bile duct ligation model in mice, they observed that L. acidophilus downregulated cholesterol 7α-hydroxylase and restored key regulators FGF15 and SHP in the ileum. This lowered overall bile acid overproduction while boosting bile salt hydrolase activity in the gut to reduce toxic, conjugated bile acids. The results support L. acidophilus as a promising probiotic to protect against cholestatic injury.

Protocatechuic acid/sodium alginate multilayer coating induced by metal ion enhanced the ulcerative colitis alleviations of *Lactiplantibacillus plantarum*

Ren and colleagues in INTERNATIONAL JOURNAL OF BIOLOGICAL MACROMOLECULES showed that a protocatechuic acid/sodium alginate multilayer coating enhances the therapeutic effects of Lactiplantibacillus plantarum in a mouse model of ulcerative colitis. Their coating method improved probiotic survival through the gastrointestinal tract and led to higher levels of short-chain fatty acids. This, in turn, helped reduce inflammation by modulating ferroptosis-related gene expression and improving amino acid homeostasis. The findings point to novel probiotic delivery systems for managing colitis.

Cancer Metabolism, Therapy, and Immunity

These articles illustrate how tumor cells and their microenvironment rewire metabolite pathways—especially involving fatty acids, amino acids, and nucleotides—to drive growth and therapy resistance. By integrating metabolomics with functional studies, these studies reveal potential metabolic vulnerabilities, such as fatty acid uptake or ribose-5-phosphate recycling, that can be therapeutically targeted. Insights into how metabolism shapes immune evasion further illuminate strategies to enhance cancer therapies.

Targeting Fatty Acid Metabolism Abrogates the Differentiation Blockade in Preleukemic Cells

Liu and colleagues in CANCER RESEARCH showed that preleukemic hematopoietic stem cells rely on fatty acid metabolism to maintain self-renewal and evade normal differentiation. Using a conditional Runx1::Runx1t1 mouse model, they observed that AML1-ETO–expressing cells exhibited depressed oxidative phosphorylation and glycolysis but displayed an increased requirement for fatty acids. Inhibiting fatty acid uptake through either dietary deprivation or transporter knockout partially rescued normal hematopoiesis. These findings point to fatty acid metabolism as a potential target to prevent leukemic transformation.

Serum metabolomic profiling for predicting therapeutic response and toxicity in breast cancer neoadjuvant chemotherapy: a retrospective longitudinal study

Fang and colleagues in BREAST CANCER RESEARCH found that dynamic changes in serum metabolites correlate with both therapeutic responses and treatment-induced toxicities in patients undergoing neoadjuvant chemotherapy. Their untargeted metabolomic analysis revealed alterations primarily in sphingolipid and amino acid metabolism. Pre-treatment metabolite signatures, particularly certain acyl carnitines, aligned with improved treatment outcomes and hematologic tolerability. These insights could inform personalized chemo regimens for locally advanced breast cancer patients.

D-ribose-5-phosphate inactivates YAP and functions as a metabolic checkpoint

Tu and colleagues in JOURNAL OF HEMATOLOGY & ONCOLOGY showed that D-ribose-5-phosphate (D5P) operates as a metabolic checkpoint that activates YAP, allowing cancer cells to survive under glucose limitation. By tracking targeted metabolomics, they discovered that glucose deprivation lowers D5P levels, which in turn triggers YAP activation via LATS1 degradation. Activated YAP then supports purine nucleoside phosphorylase activity to restore D5P, forming a feedback loop that promotes cell viability. Supplementing D5P with glucose transporter inhibitors synergistically enhanced anti-tumor efficacy in vitro and in vivo.

CYP3A5 promotes glioblastoma stemness and chemoresistance through fine-tuning NAD+/NADH ratio

Hu and colleagues in JOURNAL OF EXPERIMENTAL & CLINICAL CANCER RESEARCH found that CYP3A5 enhances glioblastoma stemness and chemoresistance by fine-tuning the NAD+/NADH ratio. Using loss- and gain-of-function models, they showed that CYP3A5 facilitates mitochondrial fitness and promotes DNA repair via NAD-dependent enzymes like SIRT1 and PARP. Inhibition of CYP3A5 led to reduced tumorigenicity and improved sensitivity to temozolomide in mouse models. These results underscore CYP3A5 as a metabolic vulnerability in glioblastoma stem cells.

Lower respiratory tract microbiome dysbiosis impairs clinical responses to immune checkpoint blockade in advanced non-small-cell lung cancer

Zhang and colleagues in CLINICAL AND TRANSLATIONAL MEDICINE showed that lower respiratory tract microbiome dysbiosis can impair immunotherapy responses in patients with advanced non-small-cell lung cancer. Bronchoalveolar lavage fluid analyses revealed decreased

microbial diversity and distinct bacterial species in patients who did not respond well to immune checkpoint blockade. Functional studies suggested that metabolic byproducts from these bacteria influence inflammatory cytokines and chemokines, shifting the tumor immune microenvironment. Targeting local microbiota could thus enhance immunotherapeutic outcomes.

Intra-tumoral sphingobacterium multivorum promotes triple-negative breast cancer progression by suppressing tumor immunosurveillance

Mai and colleagues in MOLECULAR CANCER demonstrated that intratumoral Sphingobacterium multivorum drives triple-negative breast cancer progression by suppressing antitumor immunity. They discovered that tumor-colonizing S. multivorum promotes the recruitment of regulatory T cells, thereby inhibiting cytotoxic T-cell activity. Metabolomic profiling indicated that bacterial metabolites reshaped chemokine secretion and immune cell infiltration. This finding illuminates a potential avenue for microbiome-based therapies in aggressive breast cancers.

Exposomics and Toxicological Protection

By mapping disturbed metabolic networks in the presence of toxins like arsenic and PFAS, these studies reveal specific pathways—especially bile acids, amino acids, and lipids—that mediate toxicity. Metabolomic and exposomic screening can identify early biomarkers of organ damage and potential therapeutic agents or nutritional supplements. Such targeted interventions could mitigate the long-term impacts of environmental exposures on human and animal health.

Amelioration of arsenic-induced hepatic injury via sulfated glycosaminoglycan from swim bladder: Modulation of Nrf2 pathway and amino acid metabolism

Ou and colleagues in INTERNATIONAL JOURNAL OF BIOLOGICAL MACROMOLECULES demonstrated that sulfated swim bladder glycosaminoglycan (SBSG) reduces arsenic-induced liver injury by protecting cells from oxidative stress. In a rodent model, SBSG supplementation improved antioxidant enzyme levels and modulated ferroptosis- and detoxification-related genes via the Nrf2 pathway. Metabolomic analysis revealed that SBSG restored amino acid metabolism critical for cellular defense. This positions SBSG as a promising dietary strategy against chronic arsenic toxicity.

Chronic arsenic exposure-provoked biotoxicity involved in liver-microbiota-gut axis disruption in chickens based on multi-omics technologies

Li and colleagues in JOURNAL OF ADVANCED RESEARCH found that arsenic exposure disrupts the liver–microbiota–gut axis in chickens, leading to severe hepatic fibrosis and gut barrier dysfunction. Integrating transcriptomic, serum metabolomic, and 16S rRNA sequencing data, they showed that arsenic-induced microbiome shifts overproduced primary bile acids and compromised intestinal integrity. In turn, lipopolysaccharides from the gut circulated back to worsen liver damage. The study emphasizes how multi-omics can clarify complex host–toxin–

microbiome interactions.

Serum metabolome associated with novel and legacy per- and polyfluoroalkyl substances exposure and thyroid cancer risk: A multi-module integrated analysis based on machine learning

Wang and colleagues in ENVIRONMENT INTERNATIONAL showed that exposure to both legacy and novel PFAS correlates with increased thyroid cancer risk, possibly through disruptions in fatty acid metabolism. In a large case–control study, they employed machine learning models to identify PFHxA and PFDoA as key PFAS associated with heightened disease likelihood. Targeted metabolomics revealed that changes in lipid and amino acid pathways might underlie tumor progression. These data underscore the need for monitoring PFAS exposure and intervening in metabolic pathways to reduce thyroid cancer risk.

Microbiome and Metabolic Disease

Advanced metabolomics is illuminating how gut microbial communities shape host metabolic physiology, including liver function and obesity risk. These articles focus on key microbial metabolites—such as urolithin A and propionic acid—that influence energy balance and stress responses. Harnessing these microbe-derived metabolic signals could yield novel approaches for treating conditions like alcoholic liver disease and early childhood weight gain.

MUP1 mediates urolithin A alleviation of chronic alcohol-related liver disease via gut-microbiota-liver axis

Zhang and colleagues in GUT MICROBES showed that the gut microbial metabolite urolithin A (UA) protects against chronic alcohol-related liver disease via a microbiota–liver axis involving major urinary protein 1 (MUP1). In mice, UA reversed alcohol-induced dysbiosis and bolstered beneficial species like Akkermansia muciniphila, raising levels of propionic acid. Depleting gut microbes or performing fecal microbiota transplantation confirmed that UA's hepatoprotective effects hinged on its ability to reduce ER stress through MUP1. The findings offer insight into microbiome-targeted interventions for alcoholic liver disease.

Precocious infant fecal microbiome promotes enterocyte barrier dysfuction, altered

neuroendocrine signaling and associates with increased childhood obesity risk

Yong and colleagues in GUT MICROBES found that a distinct infant fecal microbiome profile at 1 month of age correlated with significantly higher overweight and obesity risk at 2 years. These "higher-risk" infants showed accelerated maturation of microbial taxonomy and function, alongside alterations in key neuroendocrine metabolites. In vitro assays on enterocytes exposed to microbiome extracts from these infants revealed an upregulation of obesity-linked genes and impaired epithelial barrier function. Early microbiome-based interventions may thus help lower childhood obesity rates.

Plant and Food Science

These articles showcase how pairing metabolomic and transcriptomic approaches can elucidate the biochemical underpinnings of crop performance, seed viability, and fruit preservation. By

capturing changes in amino acids, sugars, organic acids, and secondary metabolites, researchers can optimize plant growth conditions, bolster nutritional quality, and extend shelf life. Such data-driven strategies are increasingly vital for sustainable agriculture and post-harvest technologies.

Metabolomics combined with physiology and transcriptomics reveal the regulation of key nitrogen metabolic pathways in alfalfa by foliar spraying with nano-selenium

Sun and colleagues in JOURNAL OF NANOBIOTECHNOLOGY revealed that nano-selenium foliar spraying boosts alfalfa's nitrogen metabolism and photosynthesis, resulting in greater biomass and protein content. Using the 15N labeling method, they found that nano-selenium heightened the activity of key enzymes in the nitrogen assimilation pathway and increased sugar metabolites crucial for plant energy. Transcriptome and metabolome data pinpointed specific genes and metabolic pathways involved in this effect. These results highlight nano-selenium as a valuable tool for improving crop yield and nutritional quality.

The BRAHMA-associated SWI/SNF chromatin remodeling complex controls Arabidopsis seed quality and physiology

Wrona and colleagues in PLANT PHYSIOLOGY showed that the SWI/SNF chromatin remodeling complex containing BRAHMA influences seed physiology in Arabidopsis, particularly regarding dormancy and longevity. Deletion of BRM triggered altered glutathione levels and increased seed viability but also enhanced secondary dormancy. Further mechanistic work revealed that BRM directly modifies expression of the seed dormancy regulator DOG1, partly by regulating a long noncoding RNA in the DOG1 locus. The study opens new avenues for breeding seeds with optimized viability and germination profiles.

Combination transcriptomic and metabolomic reveal deterioration of the blue honeysuckle (Lonicera caerulea L.) fruit and candidate genes regulating metabolism in the post-harvest stage

Chen and colleagues in INTERNATIONAL JOURNAL OF BIOLOGICAL MACROMOLECULES demonstrated that post-harvest blue honeysuckle fruit undergoes significant quality deterioration mediated by sugar, organic acid, and flavonoid metabolism. Low-temperature storage slowed this metabolic decline, preserving fruit firmness and overall nutrient composition. Multi-omics analyses identified malic acid, naringenin, and pinobanksin as key metabolites associated with fruit senescence. These insights may help refine storage protocols to extend shelf life for this emerging berry.

Methodological Advances

Editorial Note (Metabolomics Focus):
Continuing advancements in the analytical methods underpinning small-molecule studies broaden our ability to capture metabolite dynamics in health and disease. These advancements pave the way for more precise measurements of metabolic states, which ultimately leads to more accurate and effective intervention..

Personalized Profiling of Lipoprotein and Lipid Metabolism Based on 1018 Measures from Combined Quantitative NMR and LC-MS/MS Platforms

Zhao and colleagues in ANALYTICAL CHEMISTRY showed that combining quantitative NMR and LC-MS/MS platforms provides an unprecedented 1018-measure profile of lipoproteins and lipids in population-based studies. They analyzed lipoprotein subfractions, triglycerides, and cholesteryl esters at an extraordinary level of detail, uncovering distinct molecular signatures tied to cardiometabolic risk factors. Their self-organizing map approach revealed new patterns of lipid clustering predictive of atherosclerosis and other metabolic disorders. This integrative methodology stands to advance precision health analytics.

Optimised Workflows for Profiling the Metabolic Fluxes in Suspension vs. Adherent Cancer Cells via Seahorse Technology

Giglio and colleagues in INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES showed that optimizing Seahorse technology workflows allows accurate metabolic flux profiling in both suspension and adherent cancer cells. They addressed technical challenges such as plate adaptation, reagent formulation, and normalization strategies based on viable cell counts or total protein. By refining each step, they achieved consistent measurements of oxygen consumption and glycolysis across different cell types. Their protocols offer a reliable, cost-effective way to study real-time metabolic shifts in heterogeneous cancer models.

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Metabolomics Events

GRC: Metabolomics and Human Health - The Interaction Between Humans, Lifestyles and the Environment Viewed

through Metabolism

February 2 - 7, 2025

Venue: Ventura, California, USA

Metabolomics is the comprehensive study of the metabolome, the repertoire of metabolites present in cells, tissues, and body fluids. More recently, these metabolites are being implicated in the development of unhealthy ageing and diseases, positive and negative impacts of interaction with the exposome and the promotion of human health. The human metabolic profile is influenced by a number of factors including diet, genetics, environmental factors and the microbiome. Understanding the influence of these factors at a cellular and systemic level is key to deciphering the role of metabolites in human health and promotion of lifespan. In this Gordon Conference series, we highlight state of the art metabolomics technologies and how such technologies can be used to study human health. The conference will cover exciting new applications in the field such as epidemiology, cancer, nutrition, analytical chemistry and bioinformatics and translation to human benefit.

Apply now

Bits & Bites # 01: Using Advanced Lipidomics for Better Understanding of Biology

February 6, 2025

Venue: Online

Bits & Bites 2025 is a flexible learning experience tailored for busy researchers seeking condensed yet impactful sessions. This 9-part short course series will feature in-depth and diverse topics in untargeted metabolomics such as mass spectrometry applications, statistics with both MetaboAnalyst and Bayesian statistics, GNPS, and 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.

This 1st course (for 2025) is taught by Dr. Tong Shen from UC Davis and no prior knowledge or software is required. This comprehensive course dives into systems-level lipid analysis, equipping participants with the knowledge and skills needed for advanced lipidomics studies. You will learn the fundamentals of lipid biochemistry and metabolism and cutting-edge techniques for analyzing lipids using mass spectrometry. We will guide you through key considerations for lipidomics research, including how to tailor experimental approaches to address specific biological questions. The course covers every stage of the experimental pipeline, from experimental design and sample extraction to detection methodologies, quality control, lipid structural elucidation, and data analysis. You will also gain insights into state-of-the-art technologies and emerging

perspectives in the field. Designed for both practicality and depth, this course ensures you can achieve reliability and accuracy in your lipidomics research while advancing your scientific expertise.

Check for more details

MANA SODAMeet

February 11, 2025

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 # 02: From Sample to Signal: Learn Best Practices in LC-MS for Metabolomics

February 20, 2025

Venue: Online

This course is taught by Dr. Uri Keshet from UC Davis and no prior knowledge or software is required. This course offers a comprehensive introduction to liquid chromatography-mass spectrometry (LC-MS) for metabolomics, covering both targeted and untargeted approaches. Participants will gain insights into LC-MS instrumentation, troubleshooting, and best practices for sample preparation, method development, and data analysis. Key topics include principles of sample preparation, quality management, method validation, selecting columns and solvents, optimizing gradients and flows, and employing DDA acquisition mode. Designed for researchers new to LC-MS or seeking to enhance their expertise, this course provides practical knowledge to improve the use of this powerful technique in metabolomics research.

Check for more details

MANA SODAMeet

April 8, 2025

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

6th Annual Canadian Metabolomics Conference (CanMetCon) 2025

April 24 - 25, 2025

Venue: Montreal, QC, Canada

The 6th Canadian Metabolomics Conference (CanMetCon) 2025 will be held at New Residence Hall, McGill University, Montreal, Quebec on April 24th–25th.

This year's theme, **"Clinical Metabolomics,"** highlights the growing role of metabolomics in healthcare and research. The Day 2 program will focus on four key areas:

- Clinical Metabolomics
- Computational Metabolomics and Machine Learning
- Nutrition and Health
- Public Health and Population Metabolomics

To kick off the conference, two hands-on workshops "Comprehensive Clinical Omics - From Sample to Result" will be held on April 23, led by Dr. Christoph Borchers and Dr. Jianguo (Jeff) Xia.

Workshop Part 1: Attendees will have the opportunity to train at the Warren Y. Soper Clinical Proteomics Centre, one of Canada's only certified clinical metabolomics laboratories, on the latest techniques in clinical mass spectrometry analysis and data generation.

Workshop Part 2: Participants will learn how to explore this dataset and generate diagnostic insights, with MetaboAnalyst and OmicsAnalyst, two of the most-used and most-cited data analysis tools in metabolomics and multi-omics.

Early-bird Registration Deadline - **February 28, 2025**
Abstract Submission Deadline - **March 1, 2025**

Registration is open

EMBL-EBI Introduction to Metabolomics Analysis Course

May 20 - 23, 2025

Venue: Hinxton, United Kingdom

This course will provide an introduction to metabolomics through lectures and hands-on sessions, using publicly available data, software, and tools. Participants will become familiar with standardized workflows as well as with the current state of experimental design, data acquisition (LC-MS, MS imaging), processing, and modelling. In addition, they will learn about community standards and sharing in metabolomics, particularly through the use of EMBL-EBI's MetaboLights repository and Galaxy infrastructure. Participants will learn through hands-on tutorials to use tools available for data analysis and data submission. Additionally, case studies will be discussed to show how to employ the week's learning.

Applications close on **February 2, 2025**

Check for more details

21st Annual Conference of the Metabolomics Society Metabolomics 2025

June 22 - 26, 2025

Venue: Prague, Czech Republic

21st Annual International Metabolomics Conference of the Metabolomics Society will be held on June 22-26, 2024 in Prague, Czech Republic. The conference will follow the same pattern as previous years, with Workshops on Sunday and Monday, and the full conference beginning on Monday afternoon and running through Thursday afternoon.
Scientists in academia, government, industry, and others working in the field of metabolomics are invited to submit abstracts in the following scientific themes:

- Metabolomics and Lipidomics in Health and Disease
- Plants, Food, Environment and Microbes
- Technology Advancements
- Computational Metabolomics, Statistics & Bioinformatics

Oral Abstract Submission Deadline - **March 6, 2025**
Poster Abstract Submission Deadline - **May 15, 2025**

Check for more details

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

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Metabolomics Jobs

Metabolomics Jobs

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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
16 PhD positions in Doctoral Training Unit	University of Luxembourg, Luxembourg Institute of Health, and Luxembourg Institute of Science and Technology	Luxembourg	University of Luxembourg
Post-Doctoral Position in Stem Cell Metabolomics	Université Catholique de Louvain (UCL)	Brussels, Belgium	Metabolomics Society
Metabolomics Senior Research Associate	Berkeley Lab's (LBNL) Environmental Genomics and Systems Biology (EGSB) Division	Bay Area, California, United States	Berkeley Lab
Post Doctoral Fellow in Clinical Exposomics	Emory University	Atlanta, GA, United States	Emory University

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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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