MetaboNews

This month in metabolomics

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Perspectives

Dr. Richard Lehner

Dr. Lehner started his undergraduate education in chemistry at the University of Chemistry and Technology in Prague and completed his BSc in chemistry and biochemistry and obtained his PhD in lipid biochemistry at the University of Toronto. He then pursued postdoctoral training in France and at the University of Alberta. Dr. Lehner became a faculty member at the University of Alberta in 1998. He is currently professor in the Department of Pediatrics, as well as adjunct professor in the Department of Cell Biology. Dr. Lehner is a member of national peer review committees and of several international advisory committees and boards of scientific journals concerned with lipid and lipoprotein research. Dr. Lehner's main research interests lie in the regulation of hepatic fat storage and metabolism and identification of novel therapeutic targets for lowering hepatic and blood lipid levels. Dr. Lehner has been recognized for his research nationally and internationally (Pfizer Cardiovascular Research Award, Harvard Medical School Anna Lee Memorial Lectureship, Canadian Lipoprotein Conference Simon Pierre Noel Lectureship). His research is currently funded by grants from CIHR and NSERC.

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1. How did your research on hepatic lipid metabolism lead you into the metabolomics space, and at what point did metabolomic approaches become central to your work?

Well, my involvement in metabolomics and lipidomics started well before the term metabolomics (late 1990s) and lipidomics (early 2000s) were coined. I did my PhD training at the University of Toronto under the tutelage of Dr. Arnis Kuksis, who was one of the pioneering lipidomics researchers. More than 60 years ago, Dr. Kuksis was the first to resolve molecular species of triacylglycerols by gas chromatography (GC) and not much later after this he

also established GC/MS and LC/MS methods for total lipid profiling of plasma and tissues. My PhD Thesis project was to interrogate enzymology of intestinal fat absorption. I had to prepare radiolabeled lipid substrates and intermediate metabolites by chemical and enzymatic reactions to study fat absorption and synthesis pathways because the substrates and metabolic intermediates were not commercially available at that time. Purity characterization of substrates and metabolic products employed lipid extraction, thin-layer chromatography, GC, chiral-HPLC; in other words, I was exposed to both metabolomics and lipidomics platforms early in my research career. During my PhD training I also oversaw a section of a 4th year undergraduate biochemistry lab course where students used metabolomic and lipidomic approaches to analyze the pathway by which duodenal-infused deuterium-labeled ethanol is converted to fatty acids, glycerophospholipids and neutral lipids. During my independent research career, I have continued to study lipid metabolism – focusing mainly on hepatic fat synthesis and catabolism and thus lipid analysis has remained central to our research. From mid 2000s to early 2010s our research group on Molecular and Cell Biology of Lipids here at the UofA received AHFMR and CFI funding to establish a lipid analysis suite (HPLC, GC, LC/MS) that has eventually evolved into one of the FoMD-managed Core Research Facilities.

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2. From your perspective, when did metabolomics begin to gain broader prominence in the 'omics' world, and how did that shift influence your own research direction?

I will focus on lipidomics here. Prior to 2000s only a handful of lipidomic analysis reports were published in a year but by 2020 there were hundreds such reports published a year. The increased interest in metabolomics/lipidomics (after genomics, transcriptomics and proteomics) came about once researchers understood that metabolites, including lipids, are descriptors of health and disease and therefore can be used as biomarkers. However, with tens of thousands of possible lipid species, some of which are present only in miniscule amounts, the technology also had to evolve not only to resolve the species but also to be able to detect them. I must admit that in majority of our lipid metabolism studies we obtain the relevant information from quantitative HPLC and GC analysis of lipid classes. However, we needed to delve much deeper than quantitative lipid classes analysis to determine molecular species specificity of lipid metabolizing enzymes. Global lipidomic analysis allowed us to determine that a lipid degrading enzyme we were studying showed preference for releasing specific polyunsaturated fatty acids

from triacylglycerol and this helped us solve the regulatory function of this enzyme in liver cells. Currently, we plan to employ untargeted lipidomic approaches to assess changes in lipid storage under certain nutritional conditions and genetic manipulations.

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3. Reflecting on your career, what is the most valuable piece of advice you would give to a new researcher entering either metabolomics or the study of lipid metabolism?

The key is to have clear research questions and to discuss with metabolomic/lipidomic experts what technologies to employ to answer these questions. Not every lipid analysis requires expensive quantitative MS. Also, obtaining reliable lipid signature of a sample starts with sample preparation. There is no one single solvent mixture that would quantitatively extract all lipids from a biological sample. Most lipids are also subject to oxidation due to the presence of double bonds and active groups, and care must be taken during sample preparation. I would go as far as suggest that not every laboratory is equipped to perform sample preparation for lipid analysis.

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4. What advice would you give to institutions or organizations looking to integrate metabolomics into their research workflows or clinical pipelines?

Over the past few decades there has been a lot of investment into genomics (e.g. GWAS), transcriptomics (microarrays, RNAseq, etc) and proteomics (including posttranslational modifications) but it is important to note that identifying a mutation in a gene, or changes in transcription of a gene or having an enzyme at higher or lower concentration, or observation of a posttranslational modification of an enzyme may suggest but not prove functionality. Enzymes produce metabolites and therefore metabolomics and lipidomics in case of lipid metabolizing enzymes provide an important readout of cellular functions that complement genomics, transcriptomics and proteomics datasets.

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5. What are the largest barriers currently facing metabolomics as a field? Are there specific limitations that become even more pronounced when applying it to hepatic or lipid research?

Despite the increase of interest in metabolomics/lipidomics several challenges remain. It is estimated that less than 10% of the lipid species have been characterized by LC/MS. There is a high variation in metabolite/lipid concentrations in biological samples, and this causes some difficulty in quantitative analysis. For example, lipid species concentrations in plasma range from pM for some signaling lipids to mM for triacylglycerol and cholesteryl esters. Quantitative analysis is also hampered by the lack of internal standards that could be added to aid quantitation. Therefore, quantitation of some metabolites/lipids is mostly correlative or semi-quantitative rather than absolute.

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6. What role do you see for artificial intelligence and machine learning in metabolomics research — both broadly and in the context of identifying lipid signatures or disease biomarkers?

This is already ongoing. AI used lipidomics data to identify specific lipid alterations in neurodegenerative diseases, fatty liver disease, cardiovascular disease and some cancers. As more quantitative lipidomics data from patient samples become available the disease lipid signatures will become increasingly better defined and reliable.

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7. Your work on Ces1d, Ces1g, and AADAC reveals that ER-localized lipases each play distinct roles in hepatic neutral lipid metabolism. How did metabolomics help clarify those distinctions?

All three lipases can hydrolyze trioleoylglycerol in vitro (test tube). The question was, why have three or more (there are more!) lipases localized in a particular subcellular organelle catalyzing the same reaction? It was clear to us from the start that there needed to be either some additional substrate selectivity and/or specific regulation of these enzymes. We have used predominantly metabolic tracing experiments using radiolabeled precursors to define functions of these enzymes in lipid metabolism. Interestingly, it appears that fatty acids released from lipids by Ces1d are converted to ligands for nuclear hormone receptors and transcription factors which activate transcription of genes encoding enzymes involved in de novo lipogenesis. On the other hand, Ces1g has an opposing function from Ces1d. The enzyme is upregulated during the fed state and releases polyunsaturated fatty acids EPA and DHA specifically from

triacylglycerols and these fatty acids impact processing of transcription factor called SREBP1c, which regulates expression of genes encoding enzymes synthesizing palmitic acid as well as a fatty acid desaturation enzyme. The determination of such exquisite specificity was made possible through a shotgun lipidomic approach we performed in collaboration with Harald Köfeler's group in Austria. There are still questions about AADAC substrate specificity. We know it hydrolyzes long-chain triacylglycerols, diacylglycerols and cholesteryl esters, but whether it has specific chain-length and/or fatty acid desaturation selectivity remains to be determined.

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8. MASLD is a growing global health concern. How do you think metabolomics can contribute — whether mechanistically or diagnostically — to how we understand and address fatty liver disease?

Some metabolic signatures of MASLD have been already established. These include elevation of certain amino acids, bile salts, acyl-carnitines, lipids and lipoprotein sub-classes, etc. As more of such studies are carried out the biomarkers will become more defined and useful in diagnosis and potential targeted treatment.

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9. How do you see systems-level metabolomic approaches helping to untangle the overlapping but distinct roles of multiple lipases acting on the same substrates?

This approach is necessary. We used transcriptomics and proteomics to guide our interrogations. What also needs to be considered is the subcellular distribution of the enzymes. Enzymes do not work in isolations, and this includes intracellular lipases. Many lipolytic products are bona fide signaling molecules (such diacylglycerol, monoacylglycerol, phosphatidic acid, lysophosphatidic acid, ceramides, etc.), ligands (fatty acids, retinoids, oxysterols, etc.) or functional modifiers (endoplasmic reticulum cholesterol and fatty acids), hence their channeling/conversion must be tightly controlled. Also, modulation of one lipase activity can in some cases modify the expression/activity of another lipase, therefore, employing multiple approaches is often necessary to solve the role of a given lipase in energy metabolism and/or signaling.

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10. What is metabolomics not yet doing that it should be — and where do you see the field having its greatest impact in the coming years?

Single cell metabolomics is somewhat lacking behind single cells transcriptomics and proteomics. The resolution of cell-specific metabolic signatures within heterogenic cell populations will be critical for understanding how cells communicate with each other. This will move research beyond “bulk” measurements and will allow researchers to obtain answers to critical biological questions.

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11. Given your findings on ER-localized lipases, do you think therapeutic targeting of lipase activity is a realistic avenue, and how might metabolomics accelerate that path?

Yes. There has been interest from several biotech and big pharma companies to develop inhibitors against intracellular lipases, including developing an inhibitor against CES1, the human orthologue of mouse Ces1d. Eventually, if CES1 inhibitors with good pharmacokinetic properties are developed then metabolic profiling will need to be done on primary human cells/tissues and eventually in clinical trials to demonstrate that CES1 is a good drug target for metabolic diseases or cancer.

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12. What actions do you think are most crucial for growing the metabolomics field — whether in funding, infrastructure, training, or collaboration?

First and foremost, advancing technologies to enhance sensitivity and high throughput. Protocols need to be standardized to obtain quantitative accuracy and to assure reproducibility. Because of the high cost of instruments used for metabolomic/lipidomic analyses and the need for highly specialized professionals to operate these instruments and interpret the datasets the cost of analysis also somewhat limits broader uptake and translation into healthcare. Integration with other omic platforms - genomics, transcriptomics and proteomics is necessary.

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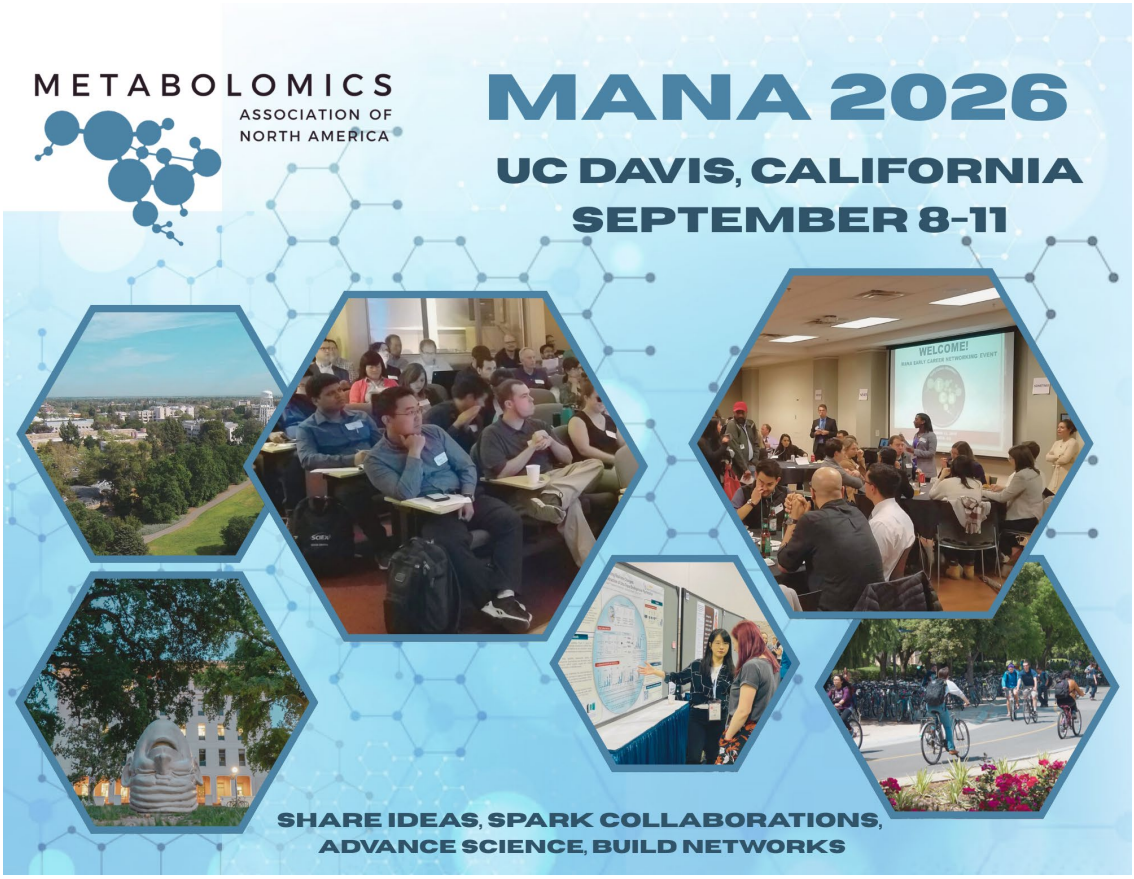
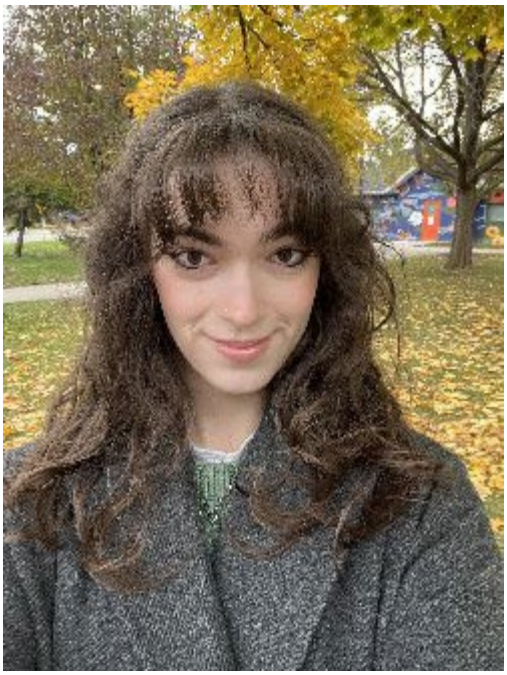


MetaboInterview

Alyss McPherson



I grew up in rural northern Ontario with my younger brother, a few dogs, several chickens, a crested gecko, and many, many, many trees. I developed a deep love for reading as soon as I figured out how, and my parents nourished that passion with a variety of books, including many on scientific topics. I became obsessed with science, at first with paleontology (because who doesn't love dinosaurs?), but the part of me that loved making bathtub potions and baking soda volcanoes eventually won out and chemistry had me hooked. I went to McMaster University for their Chemical Biology undergraduate program and graduated in 2025, then joined Dr. Joseph Okeme's research group to study chemical exposure and the "exposome" as a master's student (with the intention of soon transferring to a PhD student). Outside of research, I love fantasy and science fiction, especially the *Lord of the Rings* and *Alien* franchises, as well as all kinds of music, from metal to classical. I've taken lessons for piano and cello and played clarinet in my high school band so I can play some instruments too, though I'm a bit out of practice. I also love bread and coffee and enjoy making both, so I suppose if research doesn't work out, I can always pursue the coffee shop and bakery that so many graduate students seem to dream about!

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1. What inspired you to pursue this area of research within Metabolomics?

It was a bit of a happy accident, honestly! For a very long time, I'd actually wanted to go into medical research, and I went to McMaster for my undergrad for the Chemical Biology program as a path to medicinal chemistry. In my third year, I was struggling to find a supervisor for an undergraduate thesis until someone introduced me to Dr. Sarah Styler. She's an atmospheric and environmental analytical chemist, which was very far from my longstanding medicinal chemistry plans, but I've always been very passionate about the environment as well and she had an opportunity for me to work on a really interesting project about polycyclic aromatic hydrocarbons in Hamilton urban grime ("What's the Grime?" is the project name, for those curious!). I really enjoyed working on that project, analytical chemistry felt like a calling I just hadn't noticed yet and I appreciated how the project allowed me to interact directly with the people affected by our research. I decided I wanted to stay somewhere in that field, but I did miss the more direct connection to human health, so I applied to join Dr. Joseph Okeme's lab for graduate school. His work centres on "exposomics," which I think sits right at the intersection between environmental analytical chemistry and Metabolomics. The project I

presented on at the 27th Canadian Metabolomics Conference, comparing nontargeted chemical profiles across occupational groups, really ties together my initial passion for human health research and my newfound love for environmental and analytical chemistry.

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2. Has working in Metabolomics changed the way you think about biology, health, or disease?

Absolutely. For one, I think it has given me a deeper appreciation for just how unique every person is. I feel like most people know that we all have unique fingerprints and DNA and so on, but it wasn't until I started learning more about Metabolomics and chemical biology that I realized how the small molecules in our bodies also make us unique and how our metabolomes reflect so many parts of our biology and environment. What I've eaten lately, how much exercise I get, what places I've been, all kinds of factors are reflected in my metabolome, even if just briefly. I think I've also increasingly come to appreciate how much influence metabolites and small molecules have over health and biology. Metabolites directly regulate so many biological functions and it's really eye-opening to see just how much about the body can change based on how the small molecules in your body change. Even at just the most basic level, your body needs carbohydrates to do anything. I feel like a completely different (i.e., tired and grumpy) person when I'm too hungry and I almost instantly feel like myself again once I eat. Metabolites play a huge role in that. The body is just such an astonishingly complex system and the more I learn about Metabolomics, the more I see that complexity.

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3. How do you see your work contributing to collaboration across disciplines or research communities?

The samples for our project were collected with help from Dr. Victoria Arrandale, who's actually at the Dalla Lana School of Public Health! So, there's already some collaboration involved in this project, and I think that a project on occupational chemical exposure has a lot of potential for interdisciplinary collaboration. Chemical exposure is of course relevant to public health researchers because environmental compounds do have such a big impact on public health. Working with experts on environmental and multimedia modelling can also be very valuable to gain some insights about chemical transport in the environment and in the body, and we have some collaborators in that field with

different projects. The aim of our project is to identify how someone's workplace influences their chemical exposures, so if we identify any harmful compounds associated with a certain occupation, engineers or materials scientists might want to collaborate or at least communicate about developing alternatives. The project I presented on is still very preliminary, so it's hard to predict what collaborations are likely to actually come from it, but at the very least, I hope that projects like ours at least help to inspire interdisciplinary collaboration more broadly because we are trying to address very interdisciplinary problems.

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4. What is one thing you wish more people understood about researchers or scientific work?

I think this is a very common opinion among researchers, but I really wish more people understood what it actually means to "do your own research." That phrase gets slung around a lot and while I think there's a good sentiment to it (it is important to be skeptical and to verify information for yourself), as with a lot of sayings, it gets misused and misinterpreted. Doing scientific research is not something you can just do casually. Even doing a proper literature review takes a long time and it's not something you can do without being familiar with how science works and is communicated. If you want to know whether some food is "good" or "bad" for you (loaded terminology on its own), for instance, you can't just stop at the abstract of whatever paper you found. Scientific conclusions are often very context-specific, and you need to understand those contexts to actually make use of a conclusion. A paper may have demonstrated that a particular food is inflammatory, but under what conditions? For which populations? Was the study even in humans or did the study actually just show that a particular compound in a particular food interacts with inflammatory signalling proteins in cell lines and therefore should be further studied as a possible (but NOT definitive) cause of inflammation? And what does the rest of the literature say? I deeply believe that scientific misinformation (and disinformation) is a major factor in so many social and political issues we are facing right now, and I think that misunderstandings about how to reach and interpret scientific conclusions play a big role in the spread of misinformation.

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5. How do you think your research could translate into real-world applications?

The core of the research I am interested in is trying to better understand how

the compounds in our environments are interacting with our health. I hope that the research I contribute to can ultimately be used to protect public health from harmful chemical exposure. That might come in the form of new regulatory practices to stop certain compounds from being used. It might be through cleanup strategies to remove harmful compounds from the environment or healthcare practices to treat the effects of some exposures. However it looks exactly, in the very long term, I hope to see my research contribute to policies, innovations, and strategies that reduce the burden of chemical pollution. In the nearer future though, I think a lot of the applications of our group's research are more within the scientific community. Apart from comparing chemical profiles across occupational groups, members of our lab (myself included) work a lot on developing and applying sampling tools and methods to measure chemical exposures, which can be used by any research group interested in the same goals. For example, I've worked on a project about a method for calibrating passive air samplers with nontargeted analysis, rather than the conventional targeted analysis, so that passive air samplers can be used to measure a broader range of compounds. I hope to see other research groups apply our method to their own samplers to make passive air sampling more efficient and comprehensive.

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6. What impact do you hope your research presented at CanMetCon 2026 will have in the next few years?

I hope it helps to highlight the importance of studying nontargeted chemical profiles across occupational groups, which is still a developing field of research. We spend significant amounts of time at work and even jobs that we might think of as safe can expose us to harmful compounds, so I do think it's very important for occupational medicine to continue harnessing -omics research to understand how our workplaces might be impacting our health. I also hope it helps emphasize that so many aspects of our lifestyles and environments can impact our health and metabolome, which I think is well-recognized in general, but if someone hasn't thought before about the influence of occupation specifically on someone's metabolome, maybe my project gave them something to consider. And if occupation can impact the metabolome, maybe someone is now contemplating other demographic characteristics that might be relevant but are less studied in the literature. It's not possible for every study to include every demographic, but at the very least, I do think it's very important that we recognize how important it is to try including as many populations as possible across the field, including those we might not think of at first. So, I

hope that seeing a project about metabolomic differences by occupation inspired someone else to think about metabolomic differences in other groups of people.

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7. What trends or emerging areas in metabolomics are you most excited to follow?

I think my broader awareness of the field and its directions is still developing, but I am particularly interested in research on endocrine systems. As someone doing research on chemical exposure, I've become very aware of just how many compounds interfere with the endocrine system and how many health conditions can arise from endocrine dysregulation, whether that's caused by chemical exposure or other processes. I think Metabolomics is a useful field for studying the endocrine system, since many endocrine compounds are small molecule metabolites and many other metabolic processes are very intertwined with the endocrine system. And considering the endocrine system regulates processes throughout the entire body and is composed of several different organs, I think approaches that cast a wide net (like Metabolomics!) are really necessary for properly studying endocrine health. Especially in light of recent developments like TFA's classification as a 1B reproductive toxin and the renaming of polycystic ovarian syndrome to polyendocrine metabolic ovarian syndrome, I hope to see more research done on endocrine health, particularly at a systemic scale, and I imagine Metabolomics will have a big role to play in that research.

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8. If you could expand your project without any limitations, what would you explore next?

First, I'd really like to collect more demographic data. Since this project was a pilot study, we don't have much information on factors like age, sex, workplace seniority, diet, and so on, which can all influence the Metabolome. It would be beneficial to know more about what a participant did at work around the sampling period as well. For example, we sampled firefighters, so I'd like to know what kinds of emergencies they had responded to leading up to and during the sampling period. I'd also like to include tear fluid as an additional sample matrix, which is something I have planned for a future research project. Tear fluid is a matrix our lab group is exploring for measuring a variety of internal and external compounds, including neurochemical markers, potential

breast cancer markers, and markers of chemical exposure, and we've had some very exciting results that some of my colleagues also presented at the conference. And if I've got unlimited resources, I would love to try a blended data-dependent and data-independent acquisition approach for the sample analysis. Because we used data-dependent acquisition, which will prioritize the most abundant compounds for acquiring the MS^2 spectrum, we don't have enough spectral data for the features that were significantly different between occupational groups to assign them putative identities. It would be interesting to run the samples several times, adjusting the MS^2 acquisition parameters each time to exclude features that we already acquired MS^2 for, which I've heard about other researchers doing (possibly even at the Canadian Metabolomics Conference, though I might be mixing up conferences).

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9. Outside of research, what helps keep you motivated, creative, or balanced during demanding projects?

Playing the cello is one of my favourite hobbies. Unfortunately, I don't have as much time (or energy) for practicing as I need to play as well as I would like, but cello is my favourite instrument, and it exercises a very different part of my brain than research. Music in general keeps me going too; I think Christopher Larkin, Yo-Yo Ma, Olga Scheps, and various other composers, musicians, and ensembles deserve a spot in any acknowledgements I give at this point. Spending time with friends and loved ones keeps me sane too, of course, I enjoy playing tabletop games or having coffee or even just talking or texting with the people I care about. I also try to just take good care of myself, even when research is busy and demanding. I've found that when I sacrifice sleep or skip lunch or work without any rest, I ultimately lose more time than I gain because I just don't function as well in the long run. Even when I have to work longer hours to meet pressing timelines, I still aim to get my eight hours and three meals a day because I've learned the hard way that taking care of myself is just as much a part of my research as the writing and benchwork.

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MetaboReads

Analytical Methods & Instrumentation

Advances in measurement technology remain the engine of metabolomics progress. This month's methods papers span chromatographic optimization, software infrastructure, and multi-platform profiling workflows — from a column-cooling strategy that substantially improves HILIC separation stability, to a major update of one of the field's most widely used R packages, to new multi-tiered approaches for capturing fatty acid diversity and aging biomarkers from proteomic data. Together they reflect a field increasingly focused on reproducibility, coverage, and the practical translation of methodological gains into biological insight.

Structural Significance and Reference Value of High-Precision Coupling Constants and Raw Data in Metabolomics *Analytical Chemistry*

Giebelhaus and colleagues in *Analytical Chemistry* found that high-precision NMR coupling constants, when paired with raw spectral data, significantly improve annotation confidence in complex biological matrices. The work makes a case for standardizing the reporting of raw NMR data alongside processed outputs to support reproducible metabolite identification — a timely contribution as the field moves toward more rigorous annotation workflows.

microeco 2: A Comprehensive R Package for Downstream Analysis of Microbiome Omics Data *iMeta*

Liu and colleagues in *iMeta* found that a substantially updated version of the microeco R package — first released in 2020 and widely adopted for amplicon sequencing analysis — now includes classes for data normalization and machine learning, expanded statistical methods, improved connectivity between analysis and visualization modules, and new functions adapted from transcriptomic and metabolomic workflows. The package now handles complex abundance data from metagenomic and metatranscriptomic pipelines, broadening its utility across multi-omics study designs.

A Multi-Tiered Workflow for Examining Organic Acid Profiles Delineates Tissue-Specific Changes in Fatty Acyl Partitioning During Aging *Cell Reports Methods*

Zhou and colleagues in *Cell Reports Methods* found that a multi-tiered fatty acid profiling platform simultaneously capturing free fatty acids, esterified acyl compositions, and the total fatty acid pool within a single specimen — quantifying over 540 unique lipid and polar carboxylic acid species — revealed that aged glycolytic tissues preferentially partition odd-chain and diunsaturated fatty acids into triacylglycerols, and that aging shifts FA18:1 partitioning toward diacylglycerols over anionic phospholipids in skeletal muscle, with implications for understanding lipid-driven aging mechanisms.

ProtFI, an Efficient Frailty-Trained Proteomics-Based Biomarker of Aging, Robustly Predicts Age-Related Decline *Cell Reports Methods*

Garst and colleagues in *Cell Reports Methods* found that an ElasticNet aging biomarker trained on the Rockwood frailty index using UK Biobank Olink proteomics and metabolomics data from over 40,000 participants — designated ProteinFrailty (ProtFI) — outperformed established aging biomarkers across outcomes including incident cardiovascular disease, handgrip strength, and self-rated health, with validation confirmed in two independent Dutch cohorts, providing a systematic framework for comparing modelling choices and data sources in biological age estimation.

Low-Temperature HILIC Provides Enhanced Separations and Stability for LC-MS-Based Metabolomics *Journal of Proteome Research*

Liu and colleagues in *Journal of Proteome Research* found that cooling a zwitterionic HILIC column to 5°C substantially improves peak shape and retention time stability for untargeted LC-MS metabolomics of human plasma and cell extracts, with the resulting LT-ZHILIC method achieving high-resolution separation of 471 metabolite library standards over 100 consecutive injections. Application to glutamine- and pyruvate-deficient human cells revealed nucleotide phosphate perturbations not detected by conventional ZIC-pHILIC analysis, demonstrating the method's superior sensitivity to metabolic rewiring.

Clinical Biomarkers & Disease Metabolomics

Metabolomics is increasingly central to our understanding of disease risk, progression, and molecular heterogeneity. This month's clinical papers range from a landmark *Cell* study profiling eight omics layers across three ancestries and multiple continents, to targeted investigations of amino acid reprogramming in cancer metastasis, multi-omics tumor atlases, metabolomic aging clocks, and inflammation-linked stroke biomarkers. Collectively they illustrate the growing power of metabolomics — alone and in combination with other omics — to stratify disease risk, uncover mechanism, and point toward therapeutic intervention.

A Comparison of Deep Multiomics Profiles Across Ethnicity, Geography, and Age *Cell*

Barapour and colleagues in *Cell* found that comprehensive multiomics profiling — spanning genomics, transcriptomics, proteomics, metabolomics, lipidomics, metallomics, glycomics, and microbiomics — across 322 healthy individuals of European, East Asian, and South Asian ancestry revealed ethnicity-associated molecular features linked to host metabolism, autoimmune disease risk, drug metabolism, and neurodegenerative pathways, with geography emerging as a significant modifier of biological aging and diet–microbiome–metabolism interactions displaying distinct ethnicity-specific patterns. Published as open access, the dataset represents a substantial resource for precision medicine research.

Dysregulated Proline Metabolism Exacerbates Hepatocellular Carcinoma Metastasis via EPRS1-Mediated mRNA Translation *Cancer Communications*

Zhang and colleagues in *Cancer Communications* found that proline metabolism is enhanced during HCC metastatic progression, with L-proline directly binding glutamyl-prolyl-tRNA synthetase 1 (EPRS1) to selectively enhance translation of the invasion drivers PIK3CA, AKT3, and ITGB1. The EPRS1 inhibitor bersiporocin abolished this translational enhancement and suppressed metastasis in patient-derived orthotopic xenograft models, identifying a metabolite-driven translational mechanism as a potential therapeutic target in HCC.

A 15-Layer Multi-Omics Analysis of Gastric Cancer Ecotypes Provides Therapeutic Insights *Cell Reports Medicine*

Wang and colleagues in *Cell Reports Medicine* found that a 15-layer multi-omics atlas integrating genomics, epigenomics, transcriptomics, proteomics, post-translational modifications, protein–protein interactions, metabolomics, and microbiome profiles from 159 primary gastric adenocarcinomas defines tumor ecotypes with distinct microenvironmental architectures linked to clinical outcomes and immunotherapy response, providing a systems-level blueprint for identifying ecotype-specific therapeutic vulnerabilities in gastric cancer.

Metabolomic Ageing (MileAge) in Mid-Life Predicts Incident Vascular, Unspecified, and All-Cause Dementia *Alzheimer's & Dementia*

Mutz and colleagues in *Alzheimer's & Dementia* found that a higher metabolomic age delta (MileAge Δ — the gap between metabolite-predicted and chronological age, driven primarily by lipid, lipoprotein, and amino acid signatures) is associated with significantly higher hazard of all-cause, vascular, and unspecified dementia in 223,496 UK Biobank participants, with MileAge Δ and APOE ε4 genotype acting as independent, additive risk factors — individuals with both a high MileAge Δ and two APOE ε4 alleles faced a 10.3-fold higher dementia risk.

Metabolomic Profiles of Inflammation Associated With Incident Ischemic Stroke Risk in Women *Neurology*

Sanchez and colleagues in *Neurology* found that a 102-metabolite inflammatory signature index (i-MSI) — dominated by lysophosphatidylcholine species known to promote endothelial activation and vascular inflammation — was associated with 76% higher odds of ischemic stroke in the highest compared to the lowest quartile among women in the Nurses' Health Study, with the association for coronary heart disease confirmed independently in the Women's Health Initiative, supporting the i-MSI as a biomarker of systemic atherosclerotic risk independent of traditional cardiovascular risk factors.

Gut Microbiome–Metabolome Axis in Nutrition & Health

The gut microbiome's influence on host metabolism continues to generate high-impact findings, with metabolomics providing the functional bridge between microbial community structure and systemic health outcomes. This month's papers examine how probiotic-driven metabolic shifts in infancy can suppress antibiotic-resistant pathogens, how a single Akkermansia-derived metabolite modulates intestinal fatty acid absorption, how gut-liver metabolic crosstalk changes as fatty liver disease progresses, and how autologous fecal transplantation can restore both the infant microbiome and its metabolic fingerprint after antibiotic disruption. Together they reinforce metabolomics as the critical readout for understanding microbiome function in real biological contexts.

Metabolic Reprogramming of the Infant Gut by Bifidobacteria-Based Probiotics Drives Exclusion of Antibiotic-Resistant Pathobionts *Cell Reports Medicine*

Bargheet and colleagues in *Cell Reports Medicine* found that oral probiotic supplementation during the first four weeks of life in 152 full-term Tanzanian infants increased gut colonization by Bifidobacterium species while suppressing pathobionts including ESBL-producing Enterobacterales, with integrated metagenomics and metabolomics showing that probiotics reduced resistome load and shifted the fecal metabolome toward increased lactate and pyruvate and reduced cross-feeding pathways — changes that partially explain the reduction in antibiotic-resistant

pathobiont carriage.

Akkermansia muciniphila-Derived L-Norleucine Modulates FABP1-Dependent Fatty Acid Transport *PNAS*

Li and colleagues in *PNAS* found that intestinal FABP1 directly facilitates dietary fatty acid absorption and that the gut microbiota regulate this process through metabolites, with FABP1 protein-based metabolite enrichment coupled with untargeted metabolomics identifying L-norleucine — a major gut metabolite derived from Akkermansia muciniphila — as a competitive FABP1 inhibitor that markedly alleviates obesity in an arachidonic acid-induced model, revealing a previously unrecognized gut microbiota–FABP1 axis governing lipid homeostasis.

Gut-Liver Metabolic and Enterohormonal Remodeling Drives Progression from MASLD to Steatohepatitis *Metabolism — Clinical and Experimental*

Rivas and colleagues in *Metabolism — Clinical and Experimental* found that while cholic acid was elevated across liver, colon, and stool in both MASLD and MASH, the two disease stages differ fundamentally in their enteroendocrine response: MASLD was marked by increased circulating GLP-1, GIP, and peptide YY correlating with colonic TGR5 expression — responses absent in MASH — while MASH showed broader metabolic and lipid remodeling, elevated inflammatory cytokines, and hepatic serotonin co-localizing with fibronectin, establishing a stage-specific mechanistic map of gut-liver crosstalk in steatotic liver disease progression.

Autologous Fecal Microbiota Transplantation Restores the Infant Gut Microbiome and Metabolome After Antibiotics *mBio*

Sun and colleagues in *mBio* found that an infant who underwent autologous FMT with pre-antibiotic stool following amoxicillin treatment showed convergence toward pre-antibiotic microbiota community structure, directional restructuring of antibiotic resistance gene carriers including reduction of beta-lactam and tetracycline resistance genes, and metabolite profiles trending toward the pre-antibiotic baseline across short-chain fatty acids, bile acids, acylcarnitines, and TCA cycle metabolites — whereas a non-restored comparator infant showed persistent alteration across all three dimensions throughout follow-up.

Natural Products & Traditional Medicine

Metabolomics has become an indispensable tool for decoding the pharmacological basis of natural products and traditional herbal formulations — complex mixtures that have historically resisted mechanistic characterization. This month's papers apply integrated omics to three neurological conditions and one oncological indication, revealing how rhubarb reprograms tryptophan metabolism in ischemic stroke, how a traditional memory formulation recruits the gut microbiota to attenuate Alzheimer's pathology, how a classical patent medicine modulates metabolic pathways to relieve neuropathic pain, and how a plant alkaloid shifts cancer cell energy metabolism to

suppress tumour growth. Each study demonstrates the value of pairing metabolomics with network pharmacology, microbiome profiling, and in vivo validation to move from empirical use to molecular mechanism.

Rhubarb Ameliorates Ischemic Stroke-Induced Tryptophan–Kynurenine Metabolic Reprogramming and Neuroinflammation via IDO-1/TREM-1 *Phytomedicine*

Liu and colleagues in *Phytomedicine* found that rhubarb (Rheum officinale) restores intestinal barrier integrity and modulates tryptophan–kynurenine metabolism in an embolic MCAO stroke rat model through regulation of IDO-1 activity and suppression of the TREM-1 signaling cascade, with targeted metabolomics quantifying TRP-KYN pathway intermediates in colon and serum and surface plasmon resonance identifying bioactive constituents — including rutinum, chrysophanol glucoside, and rhein — as IDO-1 and TREM-1 inhibitors, mapping a coherent gut-to-brain metabolic axis through which rhubarb exerts neuroprotection.

Congming Decoction Alleviates Alzheimer's Disease via the Microbiota–Metabolism–Inflammation Axis *Phytomedicine*

Tang and colleagues in *Phytomedicine* found that Congming decoction (CMD) regulated 45 endogenous metabolites involved in bile acid, alpha-linolenic acid, and linoleic acid metabolism, rebalanced gut microbiota, and suppressed AKT/NF-κB-mediated neuroinflammation in Aβ25-35-induced AD rats, with antibiotic depletion abolishing these neuroprotective effects and FMT from CMD-treated donors replicating them — establishing gut microbiota as a causal mediator and demonstrating superior efficacy of the full formulation over its component herbs or herb pairs.

Pharmacological Mechanisms of Yuxuebi Tablet in Alleviating Neuropathic Pain: Network Pharmacology, 16S rRNA, and Metabolomics *Phytomedicine*

Cheng and colleagues in *Phytomedicine* found that Yuxuebi Tablet suppresses the EGFR/PI3K/AKT signalling pathway, reduces spinal inflammatory cytokines, reverses metabolic disturbances in phospholipid, amino acid, carnitine, and bile acid pathways, and modulates gut microbiota composition in a chronic constriction injury neuropathic pain rat model, with network pharmacology and molecular docking providing mechanistic grounding and 16S rRNA sequencing identifying gut microbiota shifts correlated with analgesic outcomes.

Aloperine Exerts Anti-Ovarian Cancer Effects by Regulating the TCA Cycle and Glycolysis *Journal of Ethnopharmacology*

Zhang and colleagues in *Journal of Ethnopharmacology* found that aloperine (ALO), an alkaloid from Sophora alopecuroides, increases TCA cycle intermediates (citrate, α-ketoglutarate) while suppressing glycolytic metabolites (pyruvate, lactate) in ovarian cancer cells as revealed by HPLC-MS metabolomics, simultaneously downregulating glycolytic enzymes GLUT1, PKM2, and LDHA, with molecular

docking identifying MDM2, JAK2, and CDK2 as primary protein targets and in vivo xenograft validation confirming anti-tumour activity.

Environmental Metabolomics & Exposome

Understanding how environmental chemical exposures alter human metabolism is one of the most pressing applications of metabolomics in public health research. This month's papers examine three distinct exposure contexts — ambient fine particulate matter, legacy and emerging PFAS compounds, and their reproductive consequences — using exhaled breath condensate, thermal proteome profiling, and seminal lipidomics respectively. Together they advance the case for metabolomics and lipidomics as sensitive, mechanistically informative tools for characterizing the biological effects of environmental contaminants at both the molecular and population level.

Exhaled Breath Condensate Reveals PM2.5-Driven Airway Metabolic Signature in Young Adults: A Panel Study *Environmental Science & Technology*

Song and colleagues in *Environmental Science & Technology* found that proteomic and metabolomic profiling of exhaled breath condensate (EBC) from 30 healthy young men over 35 days of ambient PM2.5 exposure (averaging 73 μg/m³) revealed consistent downregulation of six proteins including PPIA, ENO1, and HSPA8, disrupted energy metabolism and lipid homeostasis, and dose-response trends for leucine, ornithine, and phenylalanine that were reproducible across EBC, plasma, and urine — validating EBC as a minimally invasive multi-compartment biomarker matrix for real-world air pollution exposure.

Sodium p-Perfluorous Nonenoxybenzenesulfonate Directly Targets Mitochondrial Proteins to Disrupt Metabolic Cascade and Promote Nephrotoxicity *Environment International*

Lyu and colleagues in *Environment International* found that OBS (sodium p-perfluorous nonenoxybenzenesulfonate), an emerging PFAS, directly binds the mitochondrial proteins DLST and GCDH as identified by integrative thermal proteome profiling and limited proteolysis-mass spectrometry, with subsequent metabolomics showing that downregulation of these targets inhibits the TCA cycle and lysine degradation, suppresses the mitochondrial respiratory chain, reduces ATP production, and disrupts methionine metabolism — collectively driving renal injury that was mitigated by in situ overexpression of DLST and GCDH in kidney tissue.

Lipid Metabolism Links Seminal PFAS Exposure to IVF Outcomes *Environment International*

Huang and colleagues in *Environment International* found that multiple seminal PFAS species — including PFOA, PFUdA, PFDoA, PFTrDA, and 9Cl-PF3ONS — were inversely associated with high-quality embryo number in 132 men undergoing IVF, with lipidomic profiling revealing downregulation of PC–DG–PE–PS and TG–

DG–PE–PS pathways and upregulation of the PS–PE–PC pathway in men with poor outcomes, and network toxicology implicating PTDSS and PEMT as putative targets through which PFAS may disrupt male fertility-associated lipid metabolism.

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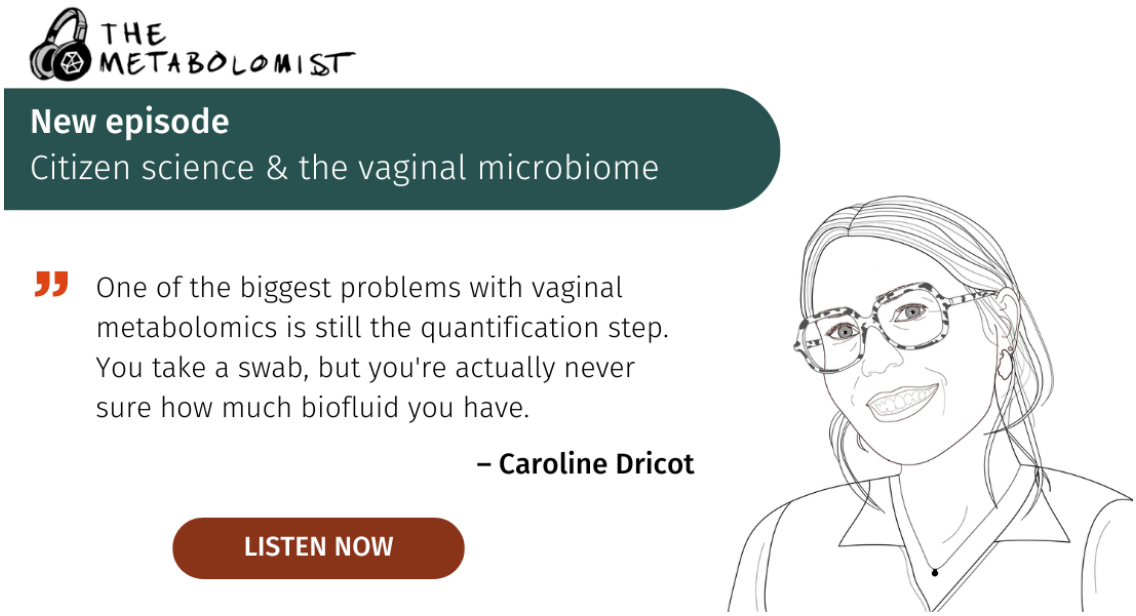
The Metabolomist



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THE METABOLOMIST

New episode
Computational metabolomics & community-driven tools

> It's the hard work of everybody listening to this podcast and beyond to report our data in such a way that it will make it possible to compare results, to compare annotations, and to really transfer knowledge and information from one experiment to another. **– Justin van der Hooft**

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Metabolomics Events

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Conference of the Metabolomics Society - Metabolomics 2026

June 21 - 24, 2026

Venue: Buenos Aires, Argentina

22nd International Conference of the Metabolomics Society, Metabolomics 2026 will be held in South America for the first time. Buenos Aires, Argentina is excited to welcome you. The conference will cover in four full days the major scientific themes of Technological Advances; Computational Metabolomics, Statistics, and Bioinformatics; Metabolomics in Health and Disease; and Metabolomics of Food, Plants, Environment, and Microbes. A special focus will highlight metabolomics for sustainable development, underscoring our collective commitment to addressing global challenges related to health, biodiversity, and environmental stewardship.

The scientific program will feature plenary and keynote lectures, parallel sessions, interactive poster presentations, and industry forums, alongside introductory and advanced workshops designed to foster learning and exchange. Complementing these academic activities, participants will be immersed in the warmth and hospitality of Latin American culture through a welcome social event, early-career gatherings, and a conference party that will celebrate the region's music, flavors, and spirit of community.

Check for more details

2026 Prague Metabolism and Signaling Symposium

June 24 - 27, 2026

Venue: Prague, Czech Republic

Discover the latest breakthroughs at the intersection of metabolism and signal transduction research. This international meeting in Prague features sessions on energy and metabolite sensing, organellar signaling, autophagy, aging, cancer, immune and stem cell metabolism, and host-pathogen interactions. Expect a diverse lineup of about 30 speakers, including two keynote addresses, covering topics from human studies to structural biology. The event also offers networking opportunities and the chance to experience beautiful Prague.

Secure your spot at the 2026 Prague Metabolism and Signaling Symposium.

Check for more details

The 1st Congress of Instrumental Analysis (CAI2026)

July 21 - 24, 2026

Venue: Salamanca, Spain

The 1st Congress of Instrumental Analysis (CAI2026) is the result of a collaboration between Spanish scientific societies to create a forum for discussion on the fundamental and applied aspects of chemical analysis. The organizing committee for this event includes the Spanish Society of Applied Spectroscopy (SEA), the Spanish Society of Chromatography and Related Techniques (SECyTA), the Spanish Society of Mass Spectrometry (SEEM), the Spanish Society of Metabolomics (SESMet), and the Spanish Society of Analytical Chemistry (SEQA).

This first meeting will integrate cutting-edge methodologies in spectroscopy, mass spectrometry, chromatography, and other related separation techniques, as well as electrochemistry. The congress aims to present both the latest advances in instrumentation and their applications in metabolomics, biomedicine, the environment, food science, and other areas of interest.

The congress aims to create a multidisciplinary forum designed to stimulate scientific exchange, foster synergies between communities, and promote the transfer of knowledge towards new analytical challenges.

Join the web seminar

MANA SODAMeet

August 11, 2026

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

MANA 2026

8th Annual Conference

September 8 - 11, 2026

Venue: UC Davis, California, USA

The Metabolomics Association of North America (MANA) is a non-profit organization that brings together a community of dedicated scientists and professionals in the field of metabolomics. With members from Canada, Mexico, and the USA, MANA is committed to fostering cooperation, coordination, and the advancement of metabolomics research in North America.

The 8th Annual MANA Conference will be hosted at the University of California. Check out the website for program information, speakers, events, registration, awards, and more.

Early-bird registration is available until **July 15, 2026.**

Check for more details

São Paulo School of Advanced Science (SPSAS) on FoodOmics

September 13 - 26, 2026

Venue: Campinas, Brazil

The São Paulo School of Advanced Science (SPSAS) on FoodOmics will be held on September 13-26, 2026, at the School of Food Engineering of the State University of Campinas (FEA-UNICAMP) in São Paulo state, Brazil.

Advances in omics sciences in areas related to food and nutrition have made it increasingly possible to understand the complexity at each layer of biological systems and at each stage of food systems, from cultivation to consumption – hence the term FoodOmics, which was established to designate the emerging interdisciplinary field that uses omics technologies to holistically understand food and nutrition, focusing on production, safety, and, above all, the benefits associated with food consumption. Thus, SPSAS on FoodOmics aims to promote discussion and deepen scientific and technological knowledge, advancing understanding of the potential of omics technologies in food science, food engineering, food technology, and nutrition.

The ten-day School's schedule combines theoretical and practical activities, including keynote lectures, poster sessions, advanced hands-on workshops, and discussion panels, all focused on foodomics and its applications. The program includes interactive sessions where participants present their research, technical visits to UNICAMP laboratories, and cultural activities.

Visit website for more details

Benelux Metabolomics Days 2026

September 22 - 23, 2026

Venue: Antwerpen, Belgium

The Benelux Metabolomics Days is the annual conference of the Benelux Metabolomics Centre (BMC), bringing together the metabolomics community from

the Netherlands, Belgium, and Luxembourg. It will take place at Stadscampus – Hof van Liere, University of Antwerp (Belgium). Hosted by Professor Wout Bittremieux and Professor Adrian Covaci, the conference will feature keynote lectures and sessions highlighting emerging and topical areas in metabolomics. Oral and poster presentations by early-career researchers will be selected through the abstract submission process.

Visit the website for more details

CMMC Symposium 2026 – Metabolic Control of Tissue Regeneration and Degeneration

September 28 - 30, 2026

Venue: Cologne, Germany

The CMMC Symposium 2026 will focus on the emerging role of metabolic programs and metabolites as key regulators of tissue regeneration and degeneration. Beyond providing energy and cellular building blocks, metabolic pathways control fundamental processes such as cell proliferation, differentiation, reprogramming and immune responses. By linking mechanistic insights with clinical perspectives, the symposium will address major challenges in molecular medicine and human disease.

We are particularly honored to welcome Elly Tanaka (IMBA, Vienna, AT), Axel Roers (University Hospital Heidelberg, DE), and Gerald I Shulman (Yale School of Medicine, US) as keynote speakers, who have also played an active role as external scientific organizers in shaping the scientific program.

The meeting is open to all and free of charge; **free registration is required**.

Visit website for more details

5th Nordic Metabolomics Conference 2026

September 28 - 30, 2026

Venue: Uppsala, Sweden

The 5th Nordic Metabolomics Conference is the official annual conference of the Nordic Metabolomics Society and will be organized at Uppsala Konsert & Kongress (UKK) in Uppsala, Sweden. The city hosts Uppsala University, who has a

longstanding tradition in Analytical Chemistry and Mass Spectrometry. The conference will host the entire depth of the metabolomics community in the Nordic Countries, high profile (inter)national speakers, will include an Early Career Event, and a dinner at Uppsala Castle.

Early bird registration deadline - **June 30, 2026**

Check for more details

MSACL 2026 16th Annual Conference & Exhibits

October 4 - 9, 2026

Venue: Montreal, Canada

MSACL's mission is to support the translation of pre-clinical research to clinical patient care. The MSACL 2026 conference will showcase cutting-edge science, address bottlenecks impeding the conversion of basic science discoveries into clinically useful applications, and equip attendees with knowledge of clinical laboratory best practices. Although the group primarily focuses on mass spectrometry, presentations and discussions on other platforms are welcome.

Early bird registration deadline - **June 30, 2026**

Check for more details

Metabolomics Jobs

Metabolomics Jobs

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Job Title	Employer	Location	Source
Research Associate (Computational Metabolomics, PostDoc)	Leibniz Institute of Plant Biochemistry	Halle, Germany	Metabolomics Society
Postdoc MALDI Imaging	University of Tübingen	Germany	Metabolomics Society
Staff Associate – LCMS Metabolomics & Exposomics	Columbia University	New York, NY, USA	Metabolomics Society
Research Associate – Environmental Analytical Chemistry	Algoma University	Sault Ste. Marie, ON, Canada	Metabolomics Society

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