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MetaboNews

This month in metabolomics

July, 2024
Vol 14, Issue 7

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

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Announcing MetaboReads

Hello, readers!

The editorial team at MetaboNews is excited to introduce an exciting change: we're rebranding our 'Recent Publications' section as 'Metaboreads'! One of the big challenges in a busy field like ours is trying to stay on top of the vast amount of papers constantly being published (for example, a quick Web of Science search for June 15 to July 15 comes up with 736 individual papers!). We're certainly aware of this - every month, in our MetaboReads section, we try to bring you a sampling of recent and intriguing papers.

With our new 'Metaboreads' feature, we're taking a more focused approach. Each month, we'll delve into the newest publications, curating a thoughtful reading list for our subscribers. Our goal is to capture a broad sampling of the incredibly diverse work going on in the metabolomics field, sort them into broadly-related research themes, and deliver you some of the high-impact papers that everyone should be reading, as well as a handful of lesser-known publications that you might find interesting. To help sift through the data, we'll also write up a quick summary and include it in the newsletter, so you can use it as a jumping-off point to really get into the new literature for the month.

We value your feedback on the feature and welcome any suggestions for improvement. Happy reading!

Michael Lowings

Editor, MetaboNews

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

Members' Corner

Board of Directors

A reflection on #MetSoc2024 and a few words of thanks

Last month many researchers descended on Osaka for the 20th Metabolomics Society conference, for science, for meeting old friends and making new ones, for some fun and karaoke, as well as for experiencing some wonderful food and culture (Osaka is after all the food capital of Japan).

As the current President of the Metabolomics Society, it was my honour to welcome our 820+ metabolomers from 50 countries around the world to Japan.

In the opening and closing ceremonies, I thanked, on behalf of the Society, many people and organizations. As a Board, we are very grateful to so many for helping us deliver such a successful and memorable meeting.

- First and foremost, our thanks go to our wonderful cochairs Prof. Eiichiro Fukusaki and Dr. Sastia Prama Putri who were our local hosts in Osaka. Thanks for bringing us to such a lovely location.
- Our meeting would not have been possible without Natasa's guidance, input and wealth of knowledge – I am personally very thankful for her continued support within the Society as the chair of our Conference Committee. Natasa, you are a star.

- Thanks also go to the conference committee, as well as the local and scientific organizing groups.
- On the ground in Osaka – and for keeping everything on track – a huge thanks to Leslie, her on-site staff and SnapIT – the Society couldn't operate without Leslie and her team who do so much hidden work in the background so we can enjoy ourselves. You are an essential part of our society.
- Finally, on the ground in Osaka are the local AV team at ATC who were just great.

In the sponsors hall, we had many sponsors. A meeting of the magnitude that the Metabolomics Society has annually could not go ahead without our sponsor's support. I and the Board of Directors are incredibly grateful to the following sponsors:

Platinum Sponsors:
Agilent, Bruker, Sciex, Shimadzu, ThermoFisher Scientific and Waters.
Gold Sponsors:
Cambridge Isotope Labs., Leco, Miltenyi Biotec and Owlstone Medical.
Silver Sponsors:
Aistl Science, AMP Inc., Avanti, Biocrates, GL Sciences, MDPI, Merck and Metwarebio.
University/Non-Profit Sponsors:
BioCyc and Riken's Centre for Sustainable Resource Science.

What is wonderful about many of these sponsors is that many come back year after year and they really make a huge difference. Thanks very much to you all.

The meeting itself was packed with great science from the workshops, from our plenary and keynote speakers to podium presentations and as well as to the posters. Every time I looked round the posters, there were people in conversation, discussing their latest and most exciting work in metabolomics. Everyone seemed to have such a nice time.

Our society are extremely appreciative of our Early Career Member Network. The EMN, headed by Silvia, hosted several events in Osaka. This included a Sunday career night with interactive round table discussions, which was very well attended, and I think many people got a lot out of these discussions. In addition, there was an EMN career workshop on Tuesday, which also included a quiz and prizes. I did hear that several more senior folks found these events to be highlights of the conference. Well done to our EMN team – we are indeed very proud of you. Or someone who is also an ECR (well, Elderly Career Member), this is especially heartwarming as these metabolomers will be guiding the future of our scientific discipline, and I feel we will be in safe hands.

In the closing ceremony, we gave the secret away and we announced that our next

conference will be in Prague and #MetSoc2025 will be hosted by Tomas Pluskal and David Friedecky. I'm already looking forward to that – especially the topic of Beeromics!

A reminder that our elections of new board members is underway and details of this can be found on the Society website – please vote in the election!

Finally, in Osaka some may remember me putting on the screen a video and picture of a 10-year-old card that Sastia gave me in Tsuruoka when I was last in Japan. For me, its message has not
withered and after the science and social aspects in Japan has blossomed even more:

Metaboromikusu daisuki

All the very best.

Roy Goodacre, University of Liverpool, UK

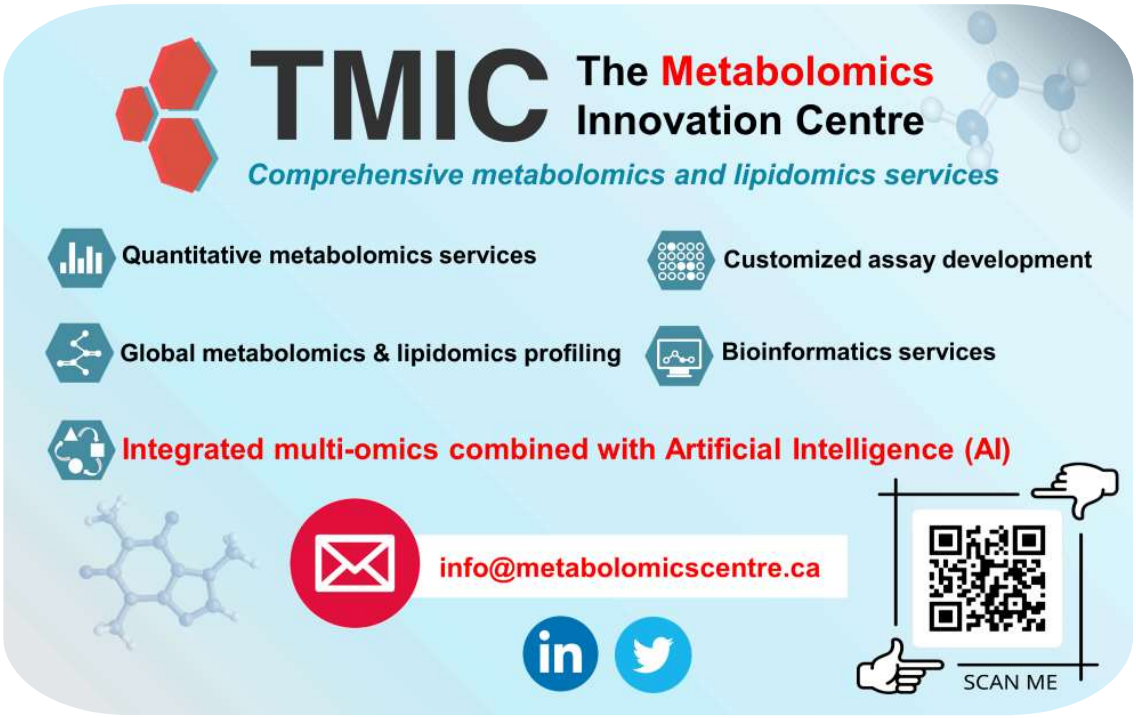
President, Metabolomics Society

TMIC proudly provides an extensive array of over 70 assays, distributed across nine nodes spanning six prominent universities. Each node is equipped with cutting-edge technology and staffed by skilled professionals dedicated to advancing omics research.

These assays cover a wide range of metabolites and analytical techniques, including targeted and untargeted approaches by using the most comprehensive set of technologies:

- NMR
- CE-MS
- GCxGC MS
- GC-MS
- LC-MS
- UPLC
- Mass Spectrometry Imaging

Also, offering customizable assays to tailor the services to best suit your needs. The assays provided are supported by TMIC's expertise in bioinformatics and statistical analysis.



Early-career Members Network (EMN)

EMN Accepting Applications!

EMN is accepting applications from enthusiastic early career metabolomics researchers starting 22nd of July until 5th of August! The applicants need to be either currently enrolled in a graduate program, or be less than 5 years from obtaining their PhD degree to be considered. In addition, applicants need to be members of the Metabolomics Society at the time of the application.

This year, we have 5 open positions. The position is for one year, with a possibility to extend for another year. Therefore, the 2-year mandate of each EMN representative will run from October 2024 to October 2026.

The application call can be found here (https://shorturl.at/ro89G). The form for the applications can be found here (https://shorturl.at/30qKt). Additionally, we specifically encourage applicants from underrepresented regions to apply including Africa, Asia, Australia/Oceania, Middle East and South America! Come join us!

Task Groups Corner

International Affiliations Task Group

The International Affiliates had a meeting on June 18, 2024, during Metabolomics 2024 in Osaka. All current affiliates were present at the meeting. Additionally, two other societies not yet affiliated at the time of the meeting, the Spanish Metabolomics Society and the Thailand Metabolomics Society, were also present. Since the meeting, the Thailand Metabolomics Society officially already became an affiliate of the Metabolomics Society.

Following the short summary of recent activities by each society, the main topic covered at the affiliates meeting in Osaka was the discussion about the “Affiliates Training Network”, an initiative first proposed at the last year’s affiliates meeting at Metabolomics 2023 and further discussed at the subsequent online meetings. The Affiliates Training Network aims to facilitate short term (3-6 months) exchanges of young scientists between the affiliate communities/laboratories. Currently, the main task to be completed over the next months is to assemble a list of laboratories interested in supporting such an exchange, and to provide up-to-date information about funding opportunities that may support such exchanges.

Lipidomics Task Group (LipidMet)

LipidMet organized a workshop “Reconnecting Lipidomics and Metabolomics for Metabolic Research“ on June 16, 2024, during Metabolomics 2024 in Osaka. The workshop, which was full to capacity, was chaired by Laura Goracci and Matej Orešič, and included three

excellent and engaging speakers, Dajana Vuckovic, Michael Witting, and Pieter Dorrestein.

The three talks and discussion focused on the similarities, differences and complementarity of lipidomics and metabolomics, from harmonization and data sharing, to applications and data analysis. The overall realization from the workshop was that the largely historical gap between the fields and communities of lipidomics and metabolomics is narrowing, and that advancements in computational mass spectrometry great opportunities for improving data harmonization and sharing practices.

LipidMet has bimonthly online meetings, which are open to all participants interested in discussing the topic. The meeting links are provided on social media (LinkedIn, X) and MetaboNews. Next online LipidMet meeting will be on September 28 at 17:00 UTC (19:00 CEST), link and program will be provided also in the next MetaboNews issue.

International Affiliates' Corner

Nordic Metabolomics Society

Visit www.nordicmetsoc.org

There are still some places available for the 4th Meeting of the Nordic Metabolomics Society is open and details can be found on: https://nmetc2024.fi/. The full program is about to be published here: https://nmetc2024.fi/scientific-programme including a large number of talks selected from submitted abstracts. The keynote speakers are:

- Professor Jingyuan Fu
- Assistant professor Maaria Kortesniemi
- Reader (Associate professor) Rodriguez-Mateos
- Researcher María Eugenia Monge
- Junior Group Leader Tomáš Pluskal
- Professor Óttar Rolfsson
- Assistant professor Egon Willighagen
- Professor Zheng-Jiang Zhu

On behalf of the local organizing committee, we are delighted to welcome you to the 4th Nordic Metabolomics Conference, an official annual conference of the Nordic Metabolomics Society. The conference aims to highlight and discuss the latest metabolomics research in the Nordic countries and abroad. The conference will be held in Biocity, University of Turku, from Monday 26th August to Wednesday 28th August. There

will be an early career researchers' event on the evening of Sunday 25th August.

The scientific programme includes five sessions focusing on different aspects of metabolomics research from method development, bioinformatics, and applications in human health and nutrition. There are 7 keynote speakers from leading international metabolomics research groups. The remainder of the talks will be selected from submitted abstracts giving the best possible platform to show case your recent metabolomics research.

The Nordic meeting will also be followed by the Biocity Symposium which is an annual event organized by Bioicity Turku and this year it will focus on metabolism in health and disease. Therefore, please join us in Turku to show case the cutting edge research in metabolomics and metabolism more generally.

On behalf of the organizing committee,
Alex Dickens, Kati Hanhineva, Matej Orešič
Co-chairs of the organising committee

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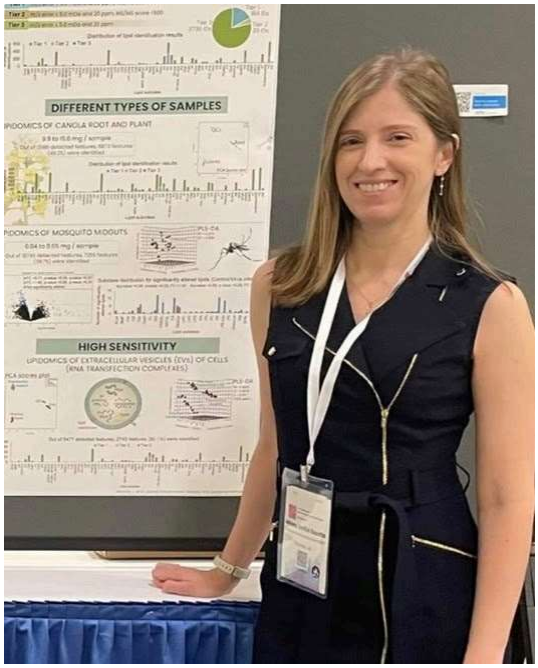
MetaboInterview

Adriana Zardini Buzatto



Assistant Professor at the University of Calgary and Associate Director of the Calgary Metabolomics Research Facility (CMRF).

Biography

Adriana is an emerging leader in lipidomics, which analyzes lipid molecules in biological fluids to investigate physiological and pathological processes. She was appointed an Assistant Professor in the Department of Biological Sciences at the University of Calgary (UCalgary) in July 2023. With a master's degree in metabolomics, a PhD in lipidomics, and industry experience, Adriana uses radical technology to address challenges in clinical and environmental research, promising a fresh and highly translational outlook on longstanding issues within the field.

How did you get involved in lipidomics?

I am an analytical chemist by training, born and raised in Brazil. I completed a Master's degree in targeted metabolomics at the University of Campinas (UNICAMP), supervised by Dr. Ana Valeria Simionato. Targeted metabolomics focuses on quantifying specific metabolites within a sample – in my case, I worked with nucleosides as potential prostate cancer biomarkers. I then started a PhD program in the same lab, aiming to work with untargeted metabolomics, which involves profiling all detectable metabolites in a sample without prior selection. This area is significantly more complex, so I needed to build my knowledge and expertise. Furthermore, research resources were quite limited in Brazil at

that time. Hence, I contacted Dr. Liang Li to discuss an internship – what we call a "sandwich PhD" in Brazil, which involves spending part of the PhD program abroad. However, Dr. Li suggested I apply for a full PhD at the University of Alberta in Edmonton. After a short visit to the facilities, I was convinced this was the right place for me. I was accepted at UofA in 2015 and started working in metabolomics. About a year into my PhD, I had the opportunity to join a Mitacs project related to lipid biomarkers of spinal cord injury. Lipids are the hydrophobic portion of our metabolome and can be used as indicators of biological states or conditions. Although they are often considered metabolites, lipids have different chemical properties and biological pathways, requiring specialized approaches (Fig. 1). The lab I was working with specialized in metabolomics, so this was an entirely new application for us. This project required lipidomics of small volumes of precious biological samples (e.g., 1-5 µL of serum and cerebrospinal fluid), a significant analytical challenge. I had to learn a lot, but this is how I found my place in lipidomics. I shifted my PhD to focus on method development and applications of lipidomics for small amounts of biological samples to investigate human diseases and processes, such as Parkinson's disease and cystic fibrosis. This involved creating and refining analytical techniques to detect and measure lipids in plasma, serum, and tissues. After graduation, I joined The Metabolomics Innovation Centre and developed their untargeted lipidomics platform, which we applied to more than 80 projects within three years. A little over a year ago, I became an Assistant Professor at the University of Calgary and recently took on the position of Associate Director of the Calgary Metabolomics Research Facility (CMRF). My lab specializes in lipidomics of biological samples, with a multidisciplinary approach connecting analytical chemistry, biochemistry, health sciences, neurosciences, microbiome studies, and data sciences. My goal is to understand complex biological processes and disease mechanisms through lipids.

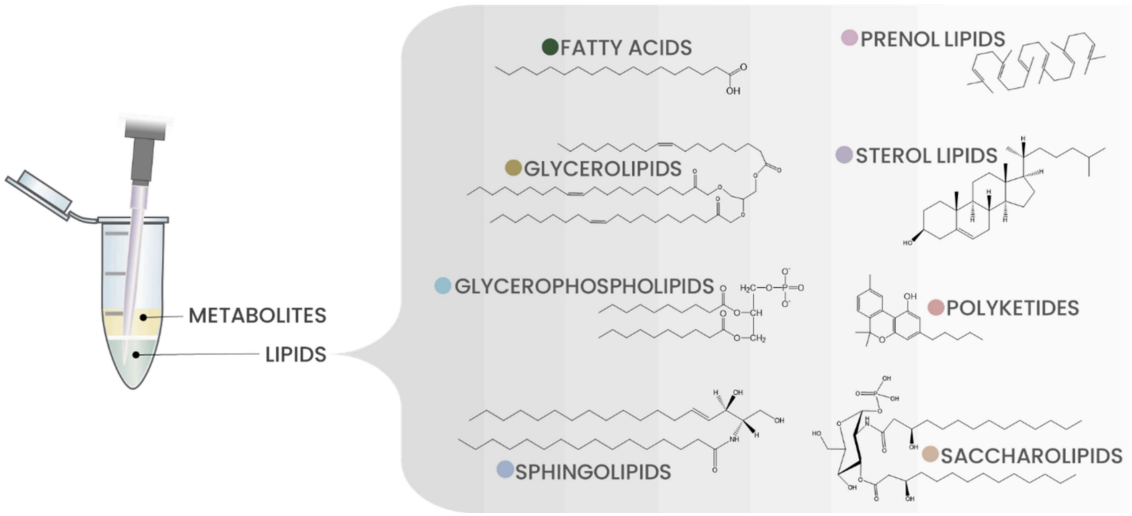


Fig. 1: Lipids can be isolated from biological samples through liquid-liquid extractions with organic solvents. The lipid fraction may contain a variety of

molecules, exemplified by representative structures within the eight major lipid categories.

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

Although lipidomics has been studied for the past 20 years, it remains an underexplored research area. Think about how much we know about the human genome or proteins - it is surprising how little we know about lipids at a detailed molecular level. We tend to think of lipids as mere energy sources, but they are involved in a variety of functions in our bodies – from forming structural membranes to participating in brain signalling pathways. We understand the main roles of lipid categories and classes (Fig. 2); for example, most of us are familiar with regular blood lipid panels done during yearly physical exams. However, more than 7,000 known molecular species can show a positive response in a clinical blood triglyceride test. When there is a disease in our body, some of those molecules could be upregulated (increased) while others are downregulated (decreased). Existing clinical tests can only show the combined effects, leading to a loss of detailed information that could be critical for early diagnosis or identifying new therapeutic targets. This is where lipidomics can make a significant difference. We have the opportunity to enhance patient diagnosis and care through detailed and comprehensive lipid analysis. Lipidomics could help us define unknown processes within and beyond the human body and develop real-world tools with practical applications to benefit the population. It is also highly versatile; lipids are present in plants, soil, bacteria, and fungi, making lipidomics an excellent tool to explore the concept of One Health – how human health is interconnected with the environment and animals. However, lipidomics requires further development before becoming a viable, reliable, and translatable tool. This is my primary focus. There is much work ahead, but lipidomics will provide crucial information to explore human health and our environment, from neurodegeneration to antibiotic resistance and even in plants and renewable energy sources.

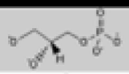
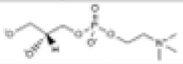
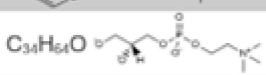
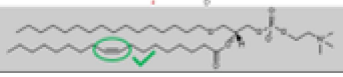
LEVEL	ANNOTATION	STRUCTURAL DEFINITION
Category	Glycero-phospholipid	
Class	PC	
Subclass	1-alkyl,2-acyl-PC	
Species	PC O-34:1	
Molecular species	PC O-16:0_18:1	
sn-positions	PC O-16:0/18:1	
Structure defined	PC O-16:0/18:1(9Z)	

Fig. 2. Lipid classification system, exemplified by the plasmenyl glycerophosphocholine PC O-16:0/18:1(9Z). Our knowledge of lipid pathways is mainly restricted to the category, class, or subclass level, but molecular and structure-defined species deeply influence metabolism.

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

My lab at the University of Calgary focuses on four essential areas: technological development, lipid biomarkers of human diseases, intercellular mechanisms, and the microbiome. First, there is a significant need for improved methodological and technical tools in lipidomics, including extended experimental databases, automated methods, and robust technology. Therefore, my team and I are developing methods and tools that are reliable, validated, and applicable in real-world settings beyond the research lab. In terms of applications, I am particularly interested in exploring lipidomics to investigate neurodegeneration. The human brain is 60% lipids, but we have yet to determine the roles of most of those molecules. Lipids could potentially be used to diagnose dementia, Alzheimer's, or Parkinson's disease years before clinical symptoms appear. Early diagnosis could allow preventive treatments to extend and improve patients' lives. Additionally, we could identify new therapeutic targets for better patient care or discover signalling pathways to enhance our understanding of brain function. Emerging evidence also suggests a connection between the microbes in our gut and our brain – known as the gut-brain axis. This area of research is actively being explored in my lab.

Furthermore, my team and I are investigating how our cells use lipids to communicate with each other through small structures called extracellular vesicles (Fig. 3). The propagation of physiological and pathological processes requires communication and the exchange of materials between cells, which are protected by lipid bilayers. Therefore, these molecules are essential to understanding how these processes occur. This research area is challenging due to the difficult isolation of these structures and their small concentrations, but there is great potential for exploring intercellular mechanisms for human health and One Health research.

Lastly, I am working on bacterial lipids and their relationship with antibiotic resistance. Untreatable infections are becoming a significant threat to humanity, and we need different approaches to combat pathogenic bacteria. Lipids may be a viable route, but they haven't been fully explored yet. Hence, we are investigating how these hydrophobic molecules act within bacteria and whether there is a correlation with infections and resistance to treatments. Although those are the primary focuses of my lab, lipidomics is very versatile. Our work extends beyond these areas through collaborations. For example, we are also

investigating the lipidome of plants and yeast for gene knockout models and pathway investigations.

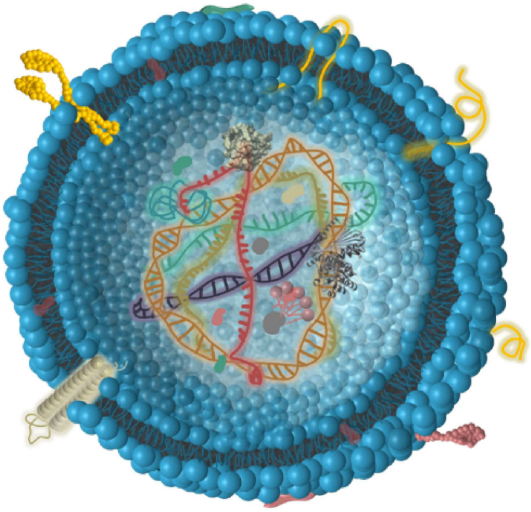


Fig. 3. Representation of an exosome, a type of extracellular vesicle. These nanometric structures are composed of proteins, genetic material, metabolites, and lipids, all involved in a lipid bilayer. They are secreted by cells and interact in a targeted manner with neighbouring cells, delivering their cargo to propagate processes.

What is happening in your country in terms of Lipidomics?

That depends on which country we consider “my country.” I have dual citizenship in Brazil and Canada. I was born and raised in Brazil, and much of my formal research training was done at the University of Campinas (UNICAMP). I owe much of my knowledge and current practices to my Brazilian professors. Although resources are not as available there, Brazilian researchers have a practical approach to science. They excel at finding new tools and creative solutions to fundamental problems with remarkable efficiency. However, funding plays a significant role in lipidomics and is more restricted there. The equipment, reagents, and standards can be costly. Still, Brazilian researchers are producing excellent science. There are outstanding researchers in Brazil – if you have a chance to work with one of them, I highly recommend it!

In Canada, we have excellent metabolomics groups exploring research lines in lipidomics. Several universities and research institutions are making significant advancements in this field. For example, I am working with the Calgary Metabolomics Research Facility (CMRF) at the University of Calgary to provide specialized knowledge and applications for lipidomics. This facility is a valuable resource for clinicians and researchers who want to explore lipids but don’t have the means or expertise to do it on their own. The University of Alberta and McMaster University also have excellent researchers investigating the role of lipids in health and disease, particularly focusing on metabolic disorders. Overall, Canada is making significant strides in lipidomics, and I intend to contribute towards making Canada a leader in this field.

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

My primary goal is to develop lipidomics platforms that can be translated into real-world applications. In other words, I aim to take my research from the lab bench to the bedside. Fundamental research is essential to get us there and is deeply needed to solve analytical and biochemical challenges, but I see the field moving more toward practical benefits for the population. Within a human health context, lipidomics can be used to create tools for early disease diagnosis and predicting disease progression years before clinical symptoms appear. This early detection could lead to preventive treatments and better disease management. Additionally, lipidomics can help identify new therapeutic targets and unravel unknown biochemical pathways, providing insights into disease mechanisms and potential therapies. Beyond human health, lipidomics has significant applications in One Health and environmental research. For example, we can use lipidomics to study plants (Fig. 4) and assess how climate changes, lack of rain, or metal toxicity affect their ability to thrive. We can develop strategies to promote better agricultural or environmental practices by understanding these mechanisms. Investigating the lipid composition of various species can help us grasp how environmental factors influence health and disease across different organisms. This knowledge can inform policies and practices that enhance the health of ecosystems and the organisms within them. Overall, lipidomics has vast potential applications. The development of robust, reliable platforms will generate valuable tools to benefit human health, agriculture, and environmental sustainability. The future of lipidomics holds great promise for improving our understanding of biological processes and addressing some of the most pressing challenges of our time.

Fig. 4. Liquid-liquid extraction of a plant sample for a lipidomics study. The bright-green layer is enriched in lipid species.

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

Its versatility. Lipids are involved in so many biological processes, making lipidomics an incredibly versatile field. We can use lipidomics to explore human health and diseases, identify new therapeutic targets, and understand the effects of microbes and diet on health. It can be applied to conservation efforts, assessing the impact of environmental stressors, and developing renewable energy sources. The possibilities are endless. This wide range

of applications highlights the strength of lipidomics, from medicine and environmental science to agriculture and energy.

What do you see as the greatest barriers for Lipidomics?

One of the most significant barriers is a lack of collaboration between researchers in different areas. Lipidomics is fundamentally multidisciplinary. We must bring together specialists from various fields, including analytical chemistry, biochemistry, cellular metabolism, microbiology, plant biology, health sciences, neuroscience, data sciences, biostatistics, and industry. This is not a research area that can be effectively tackled by one researcher or one group alone. The traditional boundaries of sciences and geography don't work in this world. Our time and resources are valuable, and as scientists, we need to share them constructively to find new answers. We also need to be more open to other approaches and ideas. A free flow of information and collaborative work between research groups is essential to achieve the full potential of lipidomics. We must adapt how we interact with our peers and disseminate our findings. Moreover, interdisciplinary collaborations will allow more innovative approaches and solutions that might not be possible within a single lab or field of study.

Another considerable barrier is research funding. Lipidomics is expensive; it requires high-end mass spectrometers, specialized chromatographic columns, ultra-pure solvents, high-quality consumables, analytical standards, etc. Our current funding practices are mostly based on grant proposals, which are often dependent on how many high-impact publications the leading PI has. Consequently, early career researchers and scientists from uncommon backgrounds sometimes suffer to fund their research, even though they may bring new views and ideas to tackle fundamental problems. We also must consider stipends for students, who often perform most of the work within a project. These academic practices are starting to change, but we need to aim for a better use of public resources.

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

Lipidomics is already taking off, but, as I mentioned before, increased collaboration and exchange of information between different areas and research groups are crucial. We have analytical chemistry groups developing methods for lipid analysis, but these methods are often not connected to biological significance. We have excellent clinicians investigating lipid species, but some of their analytical approaches may be flawed. Additionally, we use software tools adapted from metabolomics for lipidomics, but they often don't perform as needed. Consequently, scientific papers sometimes contain

significant issues, which decreases the scientific community's trust in lipidomics. Organizations such as the International Lipidomics Society and the Lipidomics Standard Initiative have made several calls for further standardization within lipidomics in the last few years with some success. However, some of the suggested standardized approaches are not freely accessible to all research groups, particularly for early-career researchers in different parts of the world. Hence, there is no consensus within the community.

On the technical side, we need platforms that are reliable, robust, easy to use, and translatable to large-scale applications. Current lipidomics methods take too much time and effort to be clinically viable. Also, they often damage delicate equipment, requiring constant maintenance and replacements – this may be suitable within a small research lab, but it doesn't work in clinical, commercial, or industrial settings. Furthermore, while we can detect thousands of compounds in biological samples, we often identify and quantify only a small percentage of them, resulting in the "dark lipidome" – a significant portion of the human and environmental lipidome that remains unknown. There are also many biomarker discovery studies with excellent potential, but we need to go beyond the discovery phase and validate our findings for clinical or environmental purposes.

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

That depends on a variety of factors, including politics. While funding opportunities exist, there is a need for a more strategic allocation of resources to generate solid benefits for the population. This means supporting projects with clear potential for real-world applications and impact beyond academic recognition. In Canada, funding is available for developing new platforms and applications, although it can be highly competitive, particularly for early-career researchers with unconventional backgrounds like myself. Funding should not be tied only to scientific publications in high-impact journals or traditional academic productivity. There are other ways to gauge a researcher's potential beyond scientific publications. Interdisciplinary and collaborative projects should be prioritized, as they can bridge the gap between different fields and enhance the overall impact of lipidomics research.

What role can lipidomics standards play?

They are essential, both from an analytical and a practical point of view. Standardization of practices has been a goal of the International Lipidomics Society for quite some time, but we are still far from achieving it. The goal here should not be to dictate how lipidomics experiments are done, as each lab has its own preferred practices, but the quantifications and annotations should be reproducible from lab to lab. Furthermore, the reporting of lipidomics datasets must follow basic principles, including details for experimental design,

lipid extraction, data collection, data processing, handling of potential contaminants, and statistics, so that the work can be fully appreciated and understood. We should be beyond publications or conference presentations where methodological aspects are unclear or not shown, but we still see this regularly. Furthermore, quality control is an essential aspect of lipidomics that should be standardized. Initiatives such as the Lipidomics Standards Initiative are valuable in this regard. Hopefully, further efforts to bring the community together will lead to advancements in standardization.

On the analytical side, using internal, isotope-labelled standards ensures the reproducibility and reliability of lipidomics experiments, which is fundamental for advancing our understanding of lipid biology and its applications in health and disease. Lipids are prone to degradation and analytical variability during experiments. We need internal standards to control these effects and ensure that our datasets have biological meaning. Absolute quantification of lipids (mol/L) is challenging due to the high complexity of our datasets, but accurate and precise absolute concentrations are necessary to define biochemical pathways. Standards are also crucial for the annotation and identification of lipid species. Experimental databases based on standards provide much better annotation accuracy than popular *in silico* (computer-predicted) databases. However, high-purity lipid standards are expensive and not widely available. Furthermore, they need to be correctly handled for high-quality databases. This is an area where organic synthetic chemists could significantly contribute to the lipidomics field by developing the standards we need to further explore lipidomes.

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

There is still much work to be done within lipidomics, but the future is bright. The potential for using lipids to advance human health and One Health is immense, and many talented people are working towards this goal. The interdisciplinary nature of lipidomics, ongoing technological advancements, and increased collaboration will certainly lead to significant breakthroughs. Furthermore, we are training the next generations of academic and industry scientists with a stronger interdisciplinary and collaborative focus. Lipidomics requires a variety of skills that can be highly complex – training, mentoring, and support are vital. Initiatives such as research hotels and exchange programs provide opportunities for young scientists from low-income countries to learn and develop their skills, as well as for a wider range of views and applications within our research approaches. I am optimistic that our efforts will result in practical applications that benefit society and enhance our understanding of complex biological processes.

I will also take this opportunity to advertise for my lab - we are staring out second year of

operations, so we are looking for graduate students with analytical, biochemical, and data sciences backgrounds and interests. Candidates are welcome to contact me for a chat.

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MetaboReads

Disease Pathogenesis and Treatment

Ongoing exploration of lipidomics and metabolomics in disease pathogenesis and treatment has yielded significant insights into how specific metabolites and lipids influence health and disease. Recent research in this topic area has focused on uncovering molecular contributions to disease processes and identifying potential therapeutic targets. This section highlights studies that demonstrate the critical roles of lipids and other metabolites in promoting tissue repair, modulating immune responses, and influencing tumor progression and circadian rhythms. These findings underscore the potential of lipidomics and metabolomics to inform novel therapeutic strategies for a range of diseases.

Oxylipins and Metabolites from Pyroptotic Cells Act as Promoters of Tissue Repair

Mehrotra et al. (Nature) discovered that the secretome from pyroptotic macrophages (Pyro-1) without IL-1beta or IL-1alpha release contains beneficial factors promoting tissue repair. Their lipidomics and metabolomics analyses identified oxylipins, particularly prostaglandin E2 (PGE2), synthesized de novo during pyroptosis, downstream of caspase-1 and cyclooxygenase-2. These factors boost migration of fibroblasts and macrophages and enhance wound healing. Pyroptotic metabolites also facilitate immune cell infiltration and polarization to CD301+ macrophages, suggesting therapeutic potential.

Cellular Spermine Targets JAK Signaling to Restrain Cytokine-Mediated Autoimmunity

Xu et al. (Immunity) highlighted spermine's role as a metabolic checkpoint that inhibits JAK1 phosphorylation by binding to its FERM and SH2 domains, impairing cytokine receptor interaction. Spermine levels are lower in systemic lupus erythematosus (SRE) patients, correlating with enhanced IFN-I signaling. Treatment with spermine and a synthesized derivative, SD1, reduced autoimmune pathogenesis in SLE and psoriasis mouse models. This study underscores spermine’s potential as an immunosuppressive treatment for autoimmune diseases.

Multi-Scale Signaling and Tumor Evolution in High-Grade Gliomas

Liu et al.(Cancer Cell) integrated proteomic, metabolomic, lipidomic, and post-translational modification data with genomic and transcriptomic measurements to map the molecular landscape of high-grade gliomas. They identified common downstream events and changes in protein interactions and glycosylation site occupancy at recurrence. Recurrent genetic alterations and phosphorylation events on PTPN11 suggest its central role in glioma progression, providing new insights for targeted therapies.

Oncogenic Fatty Acid Oxidation Senses Circadian Disruption in Sleep-Deficiency-Enhanced Tumorigenesis

Peng et al. (Cell Metabolism) demonstrated that fatty acid oxidation (FAO) senses circadian disruption in sleep-deficiency (SD)-enhanced lung tumorigenesis. Continuous increase in palmitoyl-CoA, catalyzed by ACSL1, leads to CLOCK protein stabilization through S-palmitoylation, creating a feedback loop maintaining SD-enhanced cancer stemness. Beta-endorphin, administered at dawn, can reset rhythmic expression of CLOCK and ACSL1, suggesting a chronotherapeutic strategy for SD-related cancers.

Microbiomics and Exposomics

Interactions between the gut microbiome, metabolome and exposome are increasingly recognized as pivotal factors in maintaining health and driving disease processes. This theme area explores research into alterations of the microbiome and exposome that lead to significant metabolic changes, impacting conditions such as anxiety, inflammation, renal injury, and bacterial virulence. By continuing to unearth the relationships between these three ‘omes, these studies provide valuable insights into potential therapeutic interventions for improved metabolic health.

Humid Heat Environment Causes Anxiety-Like Disorder via Impairing Gut Microbiota and Bile Acid Metabolism in Mice

Weng et al. (Nature Communications) found that a humid heat environment induces anxiety-like behavior in mice by causing gut microbiota dysbiosis and increasing serum secondary bile acids

like lithocholic acid. Neuroinflammation, indicated by elevated proinflammatory cytokines and activated PI3K/AKT/NF-kappaB signaling, was observed. Transplanting microbiota from affected mice to germ-free mice replicated these abnormalities, while Lactobacillus murinus administration reversed them, suggesting a role for probiotic administration in managing these disorders.

Gut Microbiota Dysbiosis in Hyperuricaemia Promotes Renal Injury through the Activation of NLRP3 Inflammasome

Zhou et al. (Microbiome) linked hyperuricaemia (HUA)-induced renal injury to gut microbiota dysbiosis, which promotes gut-derived uremic toxin production and NLRP3 inflammasome activation. HUA rats exhibited renal dysfunction, fibrosis, and impaired intestinal barrier functions. Faecal microbiota transplantation from HUA rats to healthy mice induced similar renal injuries. Targeting gut microbiota and the NLRP3 inflammasome may offer therapeutic strategies for renal diseases.

Enterococcus faecalis-Derived Adenine Enhances Enterohaemorrhagic Escherichia coli Type 3 Secretion System-Dependent Virulence

Martins et al.(Nature Microbiology) showed that Enterococcus faecalis increases enterohaemorrhagic E. coli (EHEC) virulence by upregulating the Type 3 Secretion System (T3SS) through adenine biosynthesis. Adenine, synthesized by E. faecalis, relieves Hha-dependent repression of T3SS gene expression in EHEC, promoting virulence. This study highlights the complexity of pathogen-microbiota interactions and their impact on gut health.

Interactions Between Intestinal Microbiota and Metabolites in Zebrafish Larvae Exposed to Polystyrene Nanoplastics: Implications for Intestinal Health and Glycolipid Metabolism

Zhu et al. (Journal of Hazardous Materials) investigated the effects of polystyrene nanoplastics (PS-NPs) on zebrafish larvae, finding that PS-NPs accumulate in the intestine, causing inflammation and oxidative stress. Disruption of intestinal microbiota and alterations in glycolipid metabolism were observed, with specific bacterial genera correlating with metabolic changes. This study highlights a putative mechanism for common industrial pollutants' negative impacts on intestinal health.

Imidacloprid-Induced Lung Injury in Mice: Activation of the PI3K/AKT/NF-κB Signaling Pathway via TLR4 Receptor Engagement

Journal: Science of the Total Environment Xie et al. established a mouse model of lung injury caused by imidacloprid (IMI), a common insecticide, showing significant impairment of pulmonary function. Metabolomics and transcriptomics analyses revealed that IMI activates the TLR4 receptor, triggering the PI3K/AKT/NF-κB signaling pathway and inducing inflammation. The study provides an insight into the mechanisms of IMI-induced pulmonary damage and a model for its mitigation.

Biomarkers and Therapeutic Targets

The identification of novel biomarkers and therapeutic targets through metabolomic research continues to transform our approach to diagnosing and treating diseases. This research topic focuses on studies that highlight the discovery of new biomarkers for conditions such as diabetic retinopathy and polymyalgia rheumatica, as well as the development of metabolomics-informed

therapeutic strategies. These advancements further underscore the value of metabolomics in enhancing our understanding of disease mechanisms and improving clinical predictivity and outcomes.

Ethanolamine as a Biomarker and Biomarker-Based Therapy for Diabetic Retinopathy in Glucose-Well-Controlled Diabetic Patients

Hu et al. (Science Bulletin) identified ethanolamine as a potential biomarker for diabetic retinopathy (DR) in glucose-well-controlled diabetic patients (GW-DR). Lower ethanolamine levels were associated with higher GW-DR risk, outperforming HbA1c as a diagnostic marker. Ethanolamine treatment in diabetic rats reduced retinal inflammation by inhibiting the DAG-dependent PKC pathway, offering a new therapeutic approach for GW-DR.

β-Hydroxybutyrate Restrains Colitis-Associated Tumorigenesis by Inhibiting HIF-1α-Mediated Angiogenesis

Huang et al. (Cancer Letters) demonstrated that β-hydroxybutyrate (BHB) inhibits tumorigenesis in colitis-associated cancer (CAC) by targeting HIF-1α/VEGFA signaling. BHB supplementation reduced tumor burden and angiogenesis in a CAC mouse model. Transcriptome analysis showed decreased VEGFA expression in hypoxic-treated cells, with HIF-1α deletion reversing BHB's effects. These findings suggest BHB as a potential preventive and therapeutic agent for colonic tumors.

Polymyalgia Rheumatica Shows Metabolomic Alterations that are Further Altered by Glucocorticoid Treatment: Identification of Metabolic Correlates of Fatigue

Manning et al. (Journal of Autoimmunity) explored metabolomic alterations in polymyalgia rheumatica (PMR) and their modification by glucocorticoid treatment. PMR and giant cell arteritis (GCA) altered metabolite signatures, with further changes seen post-treatment. Fatigue correlated with specific metabolites, including low serum glutamine, regardless of treatment, suggesting new avenues for managing persistent symptoms in PMR.

Methodologies and Techniques

Methodological advances provide the foundation for sensitive and comprehensive analyses of metabolic processes. This research topic examines the latest advancements in the field, including the application of deep learning to enhance NMR spectroscopy resolution, and the discovery of biosynthetic pathways for valuable plant metabolites. These innovations continue to advance our toolbox for understanding metabolomics, and our ability to develop applications that benefit the field and others.

Resolution Enhancement of Metabolomic J-Res NMR Spectra Using Deep Learning

Yan et al.(Analytical Chemistry) introduced J-RESRGAN, a deep learning-based method to enhance the resolution of J-Res NMR spectra. The model, trained on simulated high-resolution spectra, significantly improved peak resolution in various samples. This advancement enhances the precision of NMR-based metabolomics studies, facilitating better data interpretation and analysis.

Steroidal Scaffold Decorations in Solanum Alkaloid Biosynthesis

Lucier et al. (Molecular Plant) elucidated the biosynthetic pathways of steroidal glycoalkaloids in Solanum species, discovering 12 enzymes from Solanum nigrum involved in the conversion of cholesterol precursor to bioactive alkaloids like solasodine. They also identified enzymes in eggplant responsible for further modifications. This work offers a genetic toolbox for engineering steroidal alkaloids through synthetic biology.

Industrial and Agricultural Applications

Metabolomics is playing an increasingly vital role in industrial and agricultural applications, offering innovative solutions to enhance productivity, sustainability, and quality control. This section highlights studies that leverage metabolomic techniques to address key challenges in these sectors. Research includes the analysis of metabolite changes in insect-infested crops, the investigation of pesticide impacts on plant metabolism, and the use of microbial inoculants to improve soil health and crop yield, and selective degradation of harmful metabolites in human urine in industrial water recycling. These studies underscore the potential of metabolomics to drive advancements in industrial processes and agricultural practices, promoting both efficiency and environmental sustainability.

Metabolomics Analysis of Physicochemical Properties Associated with Quality Deterioration in Insect-Infested Hawthorn Berries

Cheng et al. (Food Chemistry) analyzed the impact of insect infestation on hawthorn berries, identifying 184 differential metabolites affected, including flavonoids and fatty acids. They highlighted uric acid and hippuric acid as biomarkers for quality deterioration. The study emphasizes the need for metabolomics in assessing food quality and detecting infestation.

Selective Degradation of Endogenous Organic Metabolites in Acidified Fresh Human Urine Using Sulphate Radical-Based Advanced Oxidation

Mehaidli et al. (Water Research) developed an advanced oxidation process using heat-activated peroxydisulphate to selectively oxidize organic metabolites in human urine while preserving urea and chloride. This method achieved over 90% activation of peroxydisulphate, degrading 43% of organic metabolites and removing 22% COD. The study supports the development of urine recycling technologies, emphasizing energy efficiency and product purity.

Non-Target Metabolomics Approach for the Investigation of the Hidden Effects Induced by Atrazine and Its Degradation Products on Plant Metabolism

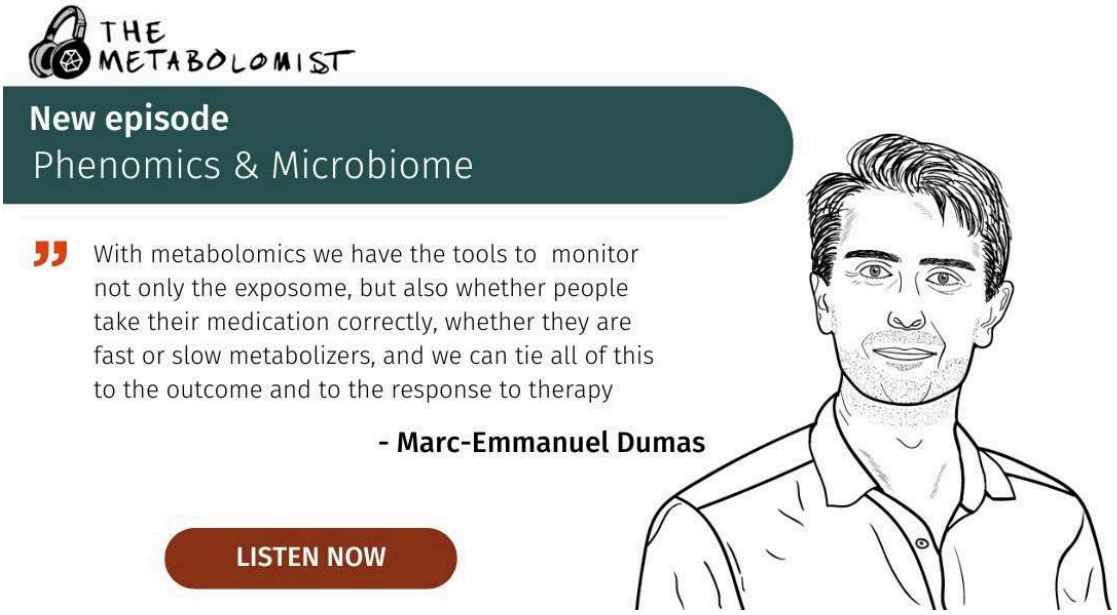
Barchanska et al. (Chemosphere) used a non-target metabolomics approach to study the effects of atrazine and its degradation products on Japanese radish metabolism. They found that atrazine and its by-products interfere with amino acid profiles and metabolic fingerprints. This approach is crucial for understanding the hidden effects of pesticides on plant health and food quality.

Integrative Analysis of Microbiome and Metabolome Revealed the Effect of Microbial Inoculant on Microbial Community Diversity and Function in Rhizospheric Soil Under Tobacco Monoculture

Lai et al. (Microbiology Spectrum) demonstrated that microbial inoculants improved soil microbiome diversity and function in tobacco monoculture. Integrative analysis showed enhanced cured leaf yield and disease resistance, with specific bacterial taxa such as Rhizobium and

Pseudomonas playing key roles. Metabolomics indicated significant effects on nicotine metabolism, providing insights into plant-microbe interactions and agricultural sustainability.

The Metabolomist Podcast



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Metabolomics Events

International Sessions in Metabolomics & Exposome Studies 2024

August 19 – 29, 2024

Venue: UC Davis Genome Center, Davis, CA, In-person

This 10-day comprehensive training course provides hands-on data analysis for untargeted metabolomics and exposome studies. It is ideal for participants with no prior experience in metabolomics, particularly those who receive, acquire, or analyze metabolomics data.

Key learning outcomes:

- Use metabolomics data to understand biochemistry and metabolism.
- Evaluate and choose the most appropriate techniques for sample preparation and data acquisition.
- Consider study design and quality control factors, including power analysis, quality, and confidence metrics.
- Gain expertise in LC-MS raw data, including challenges like in-source fragmentation and adducts
- Implement data curation best practices through hands-on exercises with metabolomics and exposome datasets.
- Develop skills in univariate and multivariate statistics, including regression analysis and Bayesian statistics.
- Mine biological information from chemical identifiers, perform pathway mapping, and conduct enrichment analysis for comprehensive data interpretation.
- Learn current compound identification methods in metabolomics, lipidomics, and exposome analyses, including MS/MS and retention time matching, in-silico tools such as MS-FINDER and SIRIUS+CSIFingerID, and utilize new resources like MassWiki.
- Understand the significance of quantification in nontargeted studies and multiomics data integration.
- Re-use existing datasets reported in Metabolomics Workbench to integrate or compare your data with prior studies

Early-bird registration fee deadline: **July 31, 2024**
The regular fee starts on **August 1, 2024.**

For more information, including registration, click here.

Learn more here

Bits & Bites # 06: Using the GNPS for Metabolomics Data Analysis and Visualizations

September 12, 2024

Venue: Online

This course is taught by Prof. Mingxun Wang, UC Riverside. The level of the course intermediate, requiring no GNPS account but no specific software or prior programming experience. In this short course, participants will get familiar with GNPS (Global Natural Products Social Molecular Networking) a web-based mass spectrometry ecosystem, and learn how to look at your data using classical molecular networking. Explore GNPS Tools for MassIVE data navigation, including classical molecular networking, data selection, mastering molecular network workflows, interactive LC/MS visualization, and compound identification. Uncover insights into intricate mass spectrometry data efficiently. Exciting material to be covered with new additions to GNPS, that will be launched in the Wang Lab in 2024.

The tuition is $175 per Bite and will take approx. 4 hours.

Check for more details

Bits & Bites # 07: Using MetaboAnalyst for Metabolomics Statistics and Data Visualizations

October 3, 2024

Venue: Online

This course is taught by Prof. Jeff Xia, McGill University. The level of the course is introductory, requiring basic computer skills and no prior programming experience is necessary. In this short course, participants will focus on mastering MetaboAnalyst 5.0, the robust platform for statistical analysis in metabolomics. Learn data input, preprocessing, and key analyses like PCA, PLS-DA, and OPLS-DA. Explore functional analysis techniques, and biomarker identification, and tackle complex metadata for robust statistical insights in metabolomics data.

The tuition is $175 per Bite and will take approx. 4 hours.

Check for more details

Metabolomics in Toxicology course

October 7 – 9, 2024

Venue: School of Biosciences - University of Birmingham, England

This 3-day course introduces the use of LC-MS based metabolomics to study toxicological processes and toxicological risk. This course provides hands-on experience for both the Q Exactive™ Plus (QE+) and Orbitrap ID-X™ Tribrid™ mass spectrometers, using a single toxicological case-study to guide delegates through an introduction to metabolomics in toxicology, from experimental design to metabolite identification.

This course is led and delivered by five experts in the field of metabolomics and includes lectures, laboratory sessions, and computer workshops to provide a detailed overview of how metabolomics can be used in toxicological research.

Early-bird registration deadline: **September 7, 2024 (terms and availability apply)**.
For more information, including registration, click here.

Learn more here

Untargeted Metabolomics LC/MS Data Processing course

October 14 – 16, 2024

Venue: School of Biosciences - University of Birmingham, England

This 3-day course is designed to address challenges associated with untargeted metabolomics data processing, and is recommended for either (i) individuals who have already completed an introductory-level BMTC course, or (ii) delegates with existing intermediate experience operating LC-MS metabolomics, and will provide trainees with furthered skills in metabolomics data processing and analytics.

Delegates will be provided with real LC-MS datasets for hands-on analysis, and throughout several sessions will be guided through various tools for metabolomic data processing and statistical analysis, including XCMS, univariate statistics, multivariate analysis, and annotation processing.

Early-bird registration deadline: **September 7, 2024 (terms and availability apply)**.
For more information, including registration, click here.

Learn more here

6th Annual Metabolomics MANA Conference

October 21 – 24th, 2024

Venue: Tampa, Florida

The 6th Annual MANA Conference, hosted by Drs. Tim Garrett and John Koomen, will take place from October 21-24, 2024, in Tampa, Florida. This year's conference features an impressive lineup of plenary speakers, including Drs. Tao Huan, Oliver Fiehn, Gina DeNicola, Patricia Scaraffia, and Julia Laskin, who will present their cutting-edge work in metabolomics.

Poster abstract submission deadline: **August 16, 2024**
Early-bird registration deadline: **August 30th, 2024**
For more information, including registration, click here.

Learn more here

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Bits & Bites # 08: Statistics in R for Metabolomics *New Course*

October 24, 2024

Venue: Online

This course is taught by Dr. Christopher Brydges from SomaLogic. The level of the course is intermediate, requiring basic knowledge of statistics, such as understanding what a t-test is and when to use one. In this short course, participants will focus on analyzing case/control study data and crafting compelling data visualizations in R. Explore R's core concepts, master data loading, and manipulation including missing data imputation. Learn essential data analysis techniques like univariate vs. multivariate approaches and delve into creating and customizing impactful graphs and plots.

Required Software: R and RStudio (Exact versions to be specified nearer the course date)

The tuition is $175 per Bite and will take approx. 4 hours.

Check for more details

2025 Metabolomics and Human Health

February 2 - 7, 2025

Venue: Ventura, California

The Metabolomics and Human Health GRC is a premier, international scientific conference focused on advancing the frontiers of science through the presentation of cutting-edge and unpublished research, prioritizing time for discussion after each talk and fostering informal interactions among scientists of all career stages. The conference program includes a diverse range of speakers and discussion leaders from institutions and organizations worldwide, concentrating on the latest developments in the field. The conference is five days long and held in a remote location to increase the sense of camaraderie and create scientific communities, with lasting collaborations and friendships. In addition to premier talks, the conference has designated time for poster sessions from individuals of all career stages, and afternoon free time and communal meals allow for informal networking opportunities with leaders in the field.

GRC Education Requirements: Undergraduates or those who have not obtained a bachelor's degree in science/engineering (or acceptable equivalent) are not eligible to apply to attend Gordon Research Conferences or Seminars.

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

Metabolomics Jobs

Metabolomics Jobs

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

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

Job Title	Employer	Location	Source
12 PhD positions in Xpose doctoral training unit (various topics)	Luxembourg Institute of Health (LIH), University of Luxembourg, Luxembourg Institute of Socio-Economic Research (LISER)	Luxembourg City or Belval, Luxembourg	Xpose, Luxembourg Institute of Health (LIH)

Data Scientist / Senior Data Scientist		Oxford, England	Metabolomics Society
Research Associate	MetaCom, Institute for Plant Biochemistry	Halle, GE, Germany	Leibniz Institute of Plant Biochemistry
Technical Core Director for LC/MS/MS, IRMS, and GMCS analyses	UT Health San Antonio	San Antonio, TX, USA	UT Health San Antonio
Post-Doc Fellowship in Cancer Epidemiology	American Cancer Society	Atlanta, GA, USA	American Cancer Society
Scientist, Research Data	University of Arizona	Tucson, AZ, USA	University of Arizona

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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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