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MetaboNews

This month in metabolomics

October, 2023
Vol 13, Issue 10

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

In This Issue

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Metabolomics Society News

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

General Enquiries

info@metabolomicssociety.org

Conference Corner

Save the Date for Metabolomics 2024!

We welcome you to Osaka, Japan for the 20th Annual Conference of the Metabolomics Society. **Metabolomics 2024** will be held at the ATC Hall, located at the Asia Pacific Trade Center, right on the beautiful bay of Osaka.

The conference will take place **June 16 – 20, 2024**. Information will be available in the

next few weeks, including the Call for Workshops and Sponsorship opportunities. Keep an eye out for announcements in November, see you in Japan!

Members' Corner

Board of Directors

Dear Society Members,

There is not much news this month, but what I have to share is nice:

The BoD were very pleased to learn that Kati Hanhineva, who is a Professor in the Food Sciences unit in the Department of Life Technologies at the University of Turku in Finland, has been re-elected to the Board of Directors of the Metabolomics Society. We look forward to continuing to work with Kati who has plans to address issues with ontology in the naming of metabolites.

Silvia Radenkovic, a postdoctoral fellow in the Department of Clinical Genomics, Mayo Clinic, Rochester, MN, USA, is our new Early-Career Members Network (EMN) committee chair. The BoD very much look forward to working with Silvia, and how we can continue to support our EMN members.

Finally, and most excitingly, the Board were delighted to learn that Fabien (our Secretary) and Caroline have welcomed a new precious member to their family. A bonnie baby boy

named Charlie was born on Wednesday 4th October, and the Board extends their warmest wishes to Fabien and his family for a bright and wonderful future.

In less exciting news, the BoD met yesterday for our monthly meeting. In addition to planning for next year's annual meeting in Osaka (16th – 20th June 2024; please note these dates), we had discussions on potential modifications to our website, how we grow and maintain our membership, as well as future education and training activities. Finally, we also agreed to provide extra support for our EMN committee members to attend our annual meetings.

All the very best.

Roy Goodacre, University of Liverpool, UK

President, Metabolomics Society

Early-career Members Network (EMN)

EMN is excited to introduce new EMN committee members for 2023-2024:

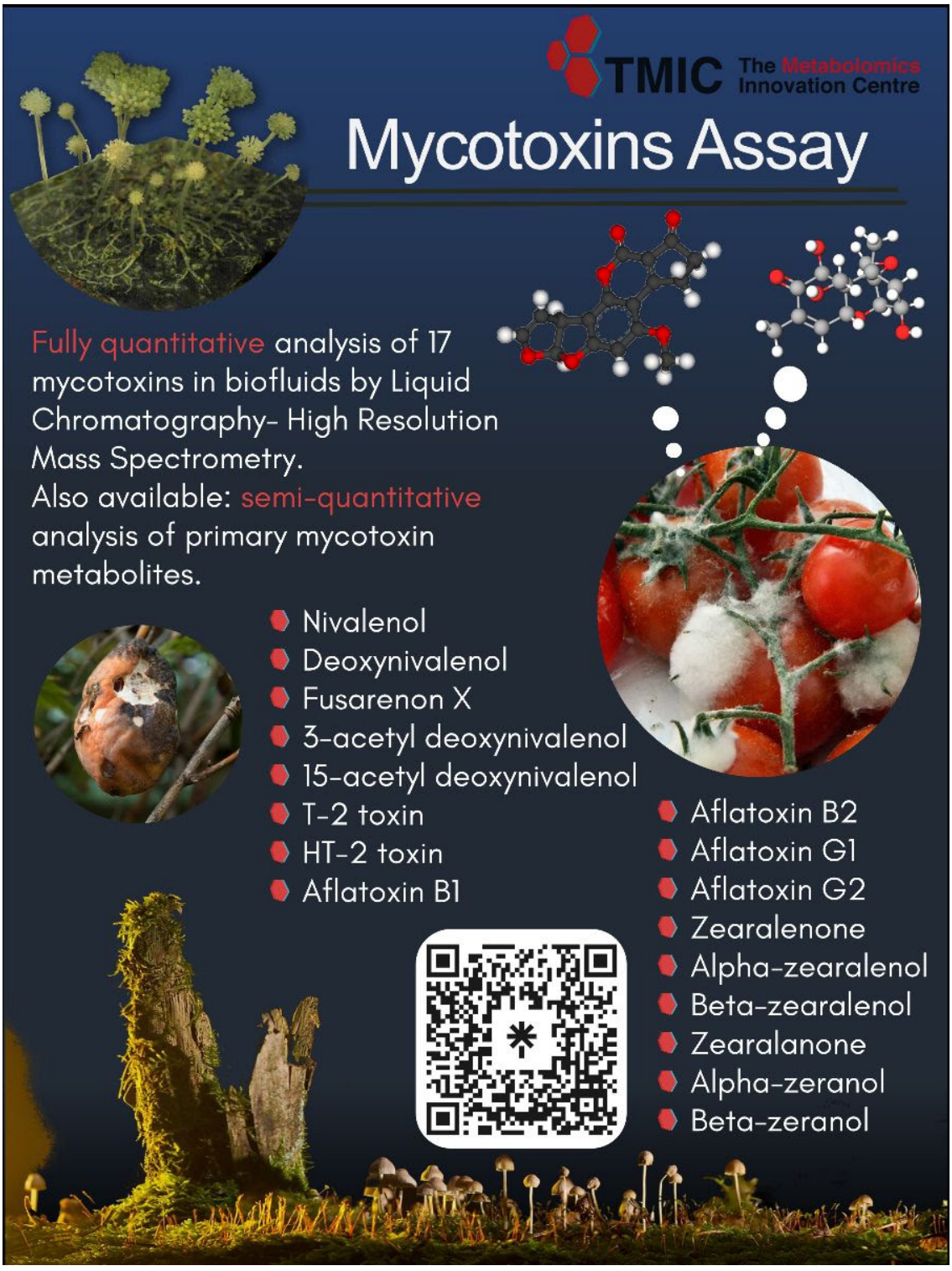
- Diana Pinto, Portugal
- Manish Kumar, India
- Monique Ryan, Australia
- Simone Zuffa, USA
- Daniela Andrea Ramirez, Argentina
- Breanna Dixon, UK
- Aleš Kvasnička, Czech Republic
- Thomas Vial, France

In addition, Silvia Radenkovic (USA) has been elected as the new chair of the EMN, while Marvin Nathanael Iman has been elected as the new secretary and Millena Barros-Santos as the EMN treasurer. The new EMN team is motivated to maintain the initiatives of the EMN and MetSoc, but also work on improving old initiatives and starting new ones. Finally, we thank all our former committee members for their contribution to EMN and MetSoc.

EMN Networking Event

The networking event for early career researchers, jointly organized by Metabolomics Society and Metabolomics Association of North America (MANA), has been rescheduled to March 2024 due to a scheduling overlap. More information regarding the event will be

shared soon, so please stay tuned for updates.



International Affiliates' Corner

Réseau Français de Métabolomique et Fluxomique (RFMF)

Visit: http://www.rfmf.fr/

The RFMF Board of Directors

You've all been looking forward to it, but the time has finally come: the renewal of the Board of Directors of the French Speaking Network in Metabolomics and Fluxomics (RFMF) and its bureau took place in July, and it's the perfect time to get out your best ties and your fanciest hats (or not)! Thanks to the RFMF members (+330), we've managed to put together a crack team to represent our wonderful organization. And for that, we thank you! And now, drum roll, here are the superheroes who will make up the brand new Board of Directors, starting with the bureau:

- Super-President: Audrey Le Gouellec - Always ready to pounce to defend the values of our organisation and solve the toughest problems.
- Vice Super-President: Pierre Pétriacq - Incredibly good at supporting the President and taking the reins when she needs them.
- Super-Treasurer: Florence Mehl - With a perfect grasp of numbers, she'll keep a close eye on the RFMF's finances and any overspending on glitter.
- Extraordinary Secretary: Justine Bertrand-Michel - Able to take notes as fast as a jogging rabbit, she'll keep track of all our incredible adventures.
- Super Events Managers (in charge of scientific communication and relations with sponsors): David Touboul - Ready to organise the most extravagant parties to celebrate our uniqueness, because we all know that we're unique and we're not all the same.

Behind this crack team, you'll also find: Cédric Bertrand, Samuel Bertrand, Benoit Colsch, Cédric Delporte, Corentine Goossens and Lindsay Peyriga. Together, we will continue to bring you more activities in the field of metabolomics and fluxomics, all in good humour and in keeping with our mantra of *Good Food, Good Science*. See you soon for some chemical adventures :) Our next scientific days will take place in the beautiful town of Saint Malo in Brittany from June 3 to 6, 2024. Don't miss the opportunity to come and visit us.

Latin American Metabolic Profiling Society (LAMPS)

Visit: https://jwist.github.io/lamps/

Celebrating the Inaugural Event: The First School of Integrated Metabolomics, 2023

In the heart of São Paulo State, from September 11-15, the Institute of Chemistry at São Paulo State University (IQ-UNESP) in Araraquara, proudly hosted the inaugural First School of Integrated Metabolomics 2023 (FSIM-2023). Spearheaded by Professors Ian Castro-Gamboa and Alan C. Pilon from NuBBE (Nucleus of Bioassays, Biosynthesis, and Ecophysiology of Natural Products), the event stitched a rich tapestry of scientific discourses and collaborations. The School was cost-free for all attendees and was endorsed by LAMPS. A unique assemblage of experts like Dr. María Eugenia Monge from CIBION-CONICET, Argentina; Dr. Mónica Cala from MetCore, UNIANDES, Colombia; Dr. Carlos Sánchez-Arcos from the Institute für Zoologie, Universität zu Köln, Germany; Dr. Fausto Carnevale Neto from Hexagon Bio, CA, USA; Dr. Ricardo Silva from the Faculty of Pharmacy, USP-RP, Brazil, and Dr. Tiago Leão from IQ-UNESP, Brazil, illuminated the event with their insights and knowledge.

Embracing themes of MS-based clinical metabolomics, QA and QC procedures in untargeted metabolomics, ion mobility, natural products, and ecometabolomics, the 2023 edition further dedicated an entire day to exploring AI, delving deep into bioinformatics and computational biology. Enthusiastically attended by 103 participants spanning from all Brazilian regions and international scholars from Uruguay, Costa Rica, and Colombia, the event became a melting pot of ideas and collaborative endeavors. Moreover, through the generous support of INCTBioNat, 8 stellar graduate students were awarded travel grants to participate in the school. In light of the resounding success and fruitful interactions emanating from this first edition, the organizers are thrilled to announce that a second school will be organized in Araraquara in 2025.

Metabolomics Association of North America (MANA)

Visit: https://metabolomicsna.org

We invite nominations for the MANA Board of Directors to serve 3-year term from 2024-2026. **Three** additional members of the Board are to be elected this year with an expected start date of January 1, 2024. We seek dynamic and hard-working individuals who will advance initiatives by which MANA will provide value to the North American metabolomics community. New board members will be expected to participate or spearhead at least one MANA interest group or committee, as well as help plan, coordinate and implement MANA events in the coming year at a monthly board meeting, with an average time commitment of 2 hours per week. Nominees are encouraged from all disciplines and sectors, including industry, government, and academia.

Nominations are due November 1; please use the following URL to submit nominations:
https://forms.gle/TSd67HMDj27srBL19

Self-nominations are welcome. Each nomination must be seconded by at least two MANA members. If you are unsure if a given colleague is a MANA member, or if you do not know any MANA members, please contact any board member directly or email mana@metabolomicsna.org and we would be happy to discuss with you and

provide a seconding nomination if appropriate.
The approximate election timeline is as follows:

- *Now – Oct 30: Nominations accepted*
- *Oct 31 – Nov 7: Nominations confirmed, candidates submit supporting information*
- *November 8: Bios and nominee statements distributed to MANA members*
- *November 8 – November 15: Voting for three new MANA Board members*
- *November 16 : Election results announced*
- *November 17: MANA Board meets with newly-elected members to nominate candidates for MANA President selected from Board members*
- *November 27: Nominees for MANA President announced to MANA membership*
- *November 27 - December 4: Voting for MANA President by MANA members*
- *December 5: New MANA President announced*

If you have any questions about the election process, please do not hesitate to contact us at mana@metabolomicsna.org.

Netherlands Metabolomics Centre (NMC)

Visit: www.metabolomicscentre.nl/

The annual **Benelux Metabolomics Days** organized by the **Netherlands Metabolomics Centre**
will be held **16 & 17 November 2023** in Utrecht, the Netherlands and is this year co-organized with the **Exposome-NL** project.

Together we will organize several break-out sessions, a poster session, and engage researchers to interact with other research fields.

The preliminary program is launched and can be found here: https://www.aanmelder.nl/benelux-metabolomics-days-2023/part_program

Find here the link to the conference website: https://www.aanmelder.nl/benelux-metabolomics-days-2023

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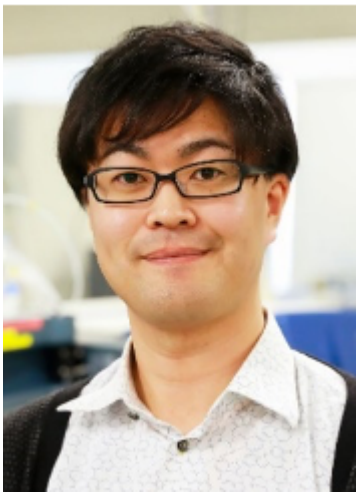
We are excited to announce that we have implemented a new format for our advertisements. However, we would like to inform you that the price is currently subject to review and may change in the near future. We encourage you to get in touch with us as soon as possible in order to freeze the current price and take advantage of this opportunity. Thank you for your continued support and we look forward to working with you.

MetaboInterview

Hiroshi Tsugawa



Assistant Professor
Tokyo University of Agriculture and Technology
System Omics Lab

Biography

I am an Associate Professor, Tokyo University of Agriculture and Technology in Japan. To date, I have worked on a field of research, computational mass spectrometry (CompMS), to deepen the understanding of complex biological system of interest (Nature Methods 2015, 2018, 2019 & Nature Biotechnology 2020). Especially, my aim is (A) to develop a data processing pipeline for complicated MS data and (B) to study mass fragmentation computationally to elucidate unknown metabolites with the proposed fragmentation

theories, achieving the global identification of metabolomes including bacterial, plant, human host, microbiota, and exposome compounds.

CompMS is an omics data science that aims to elucidate the complex biological systems using the comprehensive profile of metabolome, proteome, and glycome by converting mass spectral data to chemical structures. Importantly, MS is an essential technique for various omics sciences including metabolomics, lipidomics, proteomics, glycomics, and small RNA analyses. Thus, the innovation of CompMS has a substantial impact to various life science- and medical applications. My aim from now on is to accelerate the CompMS sciences integrating various omics layers data and imaging MS, and to conduct researches from basic biology to industrial application linking MS data to IoT society.

How did you get involved in metabolomics?

When I was a fourth-year student at Osaka University in Japan in 2009, I joined Prof. Eiichiro Fukusaki's lab that works on metabolomics studies. Our department was bioengineering and our aim was to improve the accuracy and comprehensiveness of metabolic profiling (untargeted metabolomics) by using gas chromatography coupled with mass spectrometry (GC/MS). My PhD theme was to develop a computational workflow for data processing of GC/MS datasets, and the idea is currently implemented in the MS-DIAL program. Prof. Eiichiro Fukusaki learned the workflow of GC/MS-based metabolomics from Oliver Fiehn, who was at the Max Planck Institute at that time. Therefore, I was very happy to study abroad at UC Davis in Oliver Fiehn lab in 2014. [In addition to MS-DIAL, Dr. Tsugawa has also been actively involved in the development of other software applications, including MS-FINDER (Figure 1) and MRMPROBS (Figure 2)]

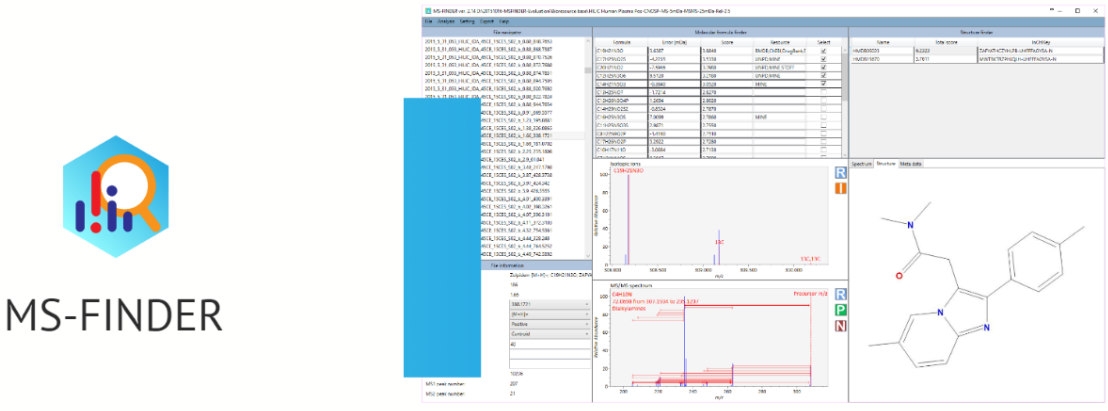


Figure 1: MS-FINDER was launched as a universal program for compound 'annotation' that supports EI-MS (GC/MS) and MS/MS spectral mining.

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

The exciting part of my research is finding novel metabolites in living organisms. For me, there are three definitions of “novel”. One is to identify a new structure that has never been reported before. The second definition is to discover a metabolite for the first time in a living organism of interest. The last one is to discover a metabolite that is associated with a phenotype. Discovering a new structure, i.e., the first definition, is very difficult. Even if the discovered metabolites are not recorded in mass spectral libraries and structure databases such as PubChem, many metabolites have already been discovered in the 20th century while they are not highlighted in biology. Nevertheless, it would be very exciting to discover new metabolites that fit one of these three definitions, and even more interesting if their biological importance could be elucidated. I believe that the continuation of untargeted metabolomics-centric science will lead to the solution of environmental issues and the establishment of a healthy and long-lived human society.

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

The Systems Biology Department, which aims to conduct a metabolomics-centric multiomics study, was established in 2021 at our university, Tokyo University of Agriculture and Technology. I became the principal investigator. Therefore, one of my tasks at this university is to let the researchers know what metabolomics can do and what can be created through research collaboration with a scientist with a unique background. Personally, I would like our faculty to become a center for metabolomics-centric systems biology in Japan.

What is happening in Japan in terms of metabolomics?

A metabolomics data repository, MetaboBank, has been established by the Foundation of the Japan Science and Technology Agency (JST). MetaboBank is a public repository for metabolomics data obtained by mass spectrometry (MS), NMR, and imaging MS. It is currently being developed in conjunction with existing public MS data repositories such as MetaboLights. In addition, a new MassBank project (Shin-MassBank) has been launched to provide both management and application of mass spectrometry data. Furthermore, a lipidome atlas project has been started as a JST-ERATO Foundation. The aim is to elucidate the mechanisms that regulate lipid diversity and its localization *in vivo* and to elucidate diseases caused by its disruption.

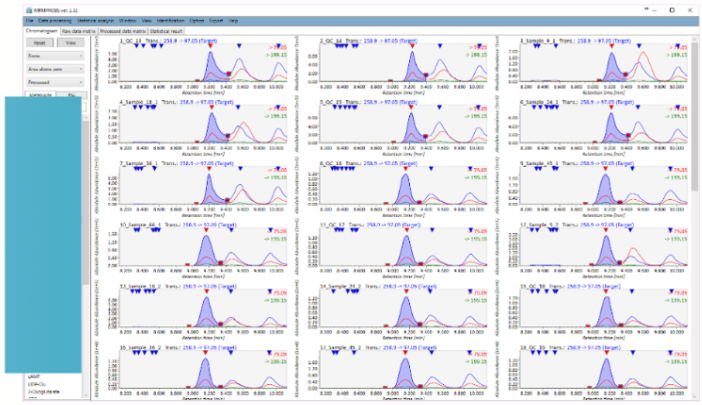


Figure 2: Another resource is MRMPROBS, launched as a universal program for targeted metabolomics using not only multiple reaction monitoring (MRM)- or selected reaction monitoring (SRM) but also SCAN and data independent MS/MS acquisition (DIA) data.

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

The goal of metabolomics, in my opinion, is to capture the diversity of metabolites that will be elucidated by integrating genomics, transcriptomics, proteomics, and the other biotechnologies. Thus, the goals of our group are (1) to develop a tool/environment to elucidate the metabolism of living organisms and (2) to elucidate the biological importance of metabolites using a multi-omics approach. To address the first issue, I keep the following two questions in mind. (A) How many metabolites can be analyzed using current methods? (B) How many cells are needed to capture the metabolome using state-of-the-art metabolomics techniques? One of our research goals is to develop biotechnology that exceeds the current benchmarks of (A) and (B). For example, the current platform of untargeted lipidomics using liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS) can annotate more than 50% of the peaks detected in blood samples, while less than 20% of the peaks are characterized in fecal samples. In addition, only 5% of the peaks detected can be annotated when natural product profiling is the scope of the research. Every research idea should be tried. Many informatics tools have recently become available and are being developed by several groups. In fact, mass spectral data has received much attention as a target for machine learning techniques. These efforts are supported and enhanced by an environment for sharing databases, spectral libraries, and source codes. Of course, some intellectual property should also be considered to make human resources stable. Most importantly for researchers, data science resources can be modified and used for research purposes.

Understanding cellular metabolism is also an emerging need in biology. Recently, with proper sample preparation and LC-MS/MS, the metabolome of a single cell can be captured. On the other hand, the use of mass spectrometry imaging (MSI) also provides

information on metabolite localization, and the spatial resolution can be achieved at the single-cell level by optimizing the instrumentation and using a mathematical approach. The advantage of LC-MS/MS based single cell metabolomics is the lower matrix effect compared to MSI. Matrix effects in MSI often give false localization information, which can be very misleading in life sciences. Therefore, data quality control in several steps is very important, such as checking the consistency of the topology in both positive and negative ion modes and multiple adduct ion forms, and validating the background effect by using internal standards. The advantage of MSI-based single-cell metabolomics is the higher scanning speed compared to single-cell LC-MS/MS techniques. In fact, MSI-based spatial metabolomics is available not only for imaging the metabolome, but also for capturing the abundance of metabolites at the single-cell level. Overall, increases in annotation rate, ion sensitivity, and throughput are needed in biology and clinical applications, and I believe they can be achieved by the updates in computational sciences.

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

The strength of metabolomics lies in its ability to directly detect the presence of metabolites and their expression levels. Although genomics and transcriptomics can predict the function of metabolite-related genes, in many cases this is only a guess. Gene and metabolite expression information can complement each other and generate new hypotheses that cannot be generated by a single omics approach. While many researchers approach life science questions from genomic and gene expression information, metabolomics researchers have the advantage where a metabolomics-centric approach is feasible to address life science questions. In addition, biomarker discovery and natural product screening are strengths of metabolomics, allowing us to perform highly sensitive and comprehensive measurements of metabolites. The discovery of a metabolite leads to the initiation of biochemical studies of genes and proteins to elucidate the biological significance of the metabolite.

What do you see as the greatest barriers for metabolomics?

My research is based on the belief that the challenges of metabolomics lie in the sensitivity for molecular detection and the annotation to illuminate the diversity of metabolomes of living organisms. All biologists are aware of these challenges and work on life science problems by optimizing sample preparations and analytical conditions in the resources we have today. Building tools to solve these problems is fun, and it is even more fun when the tools we build lead to new discoveries in the life sciences. I would like to apply the idea of 'harmonization of analytical chemistry & informatics', which includes

developments in materials engineering and analytical chemistry as well as computer science, to this metabolomics research.

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

While there are challenges for both targeted and untargeted analysis, I would like to focus my discussion on untargeted analysis. There are many issues that need to be addressed in metabolomics research if it is to be considered for widespread use, such as next-generation sequencing (NGS). Because the purpose of using metabolomics techniques depends on the biological questions, different methodologies of mass spectrometry have been used, making data standardization difficult. These problems have been recognized for more than 15 years. This means that standardization of pretreatment and analytical chemistry methods on a global level is not to be expected. Therefore, I believe that what is needed is the organization of metadata and the creation of a computational science environment that enables the estimation of analytical parameters and detectable metabolites using the metadata information. In NGS-based analysis, even novice programmers can easily perform gene expression analysis by looking at blogs or, more recently, by asking generative AI. This is because NGS provides ATGC sequence data only, and the diversity of data structures is less than in mass spectrometry-based metabolomics studies. The same is true between metabolomics and proteomics. The physical properties of the small molecules targeted by metabolomics are more diverse than those targeted by proteomics. This situation seems to be the reason why metabolomics data analysis requires extensive knowledge and know-how in biology and analytical chemistry, and metabolomics is perceived as a highly specialized method. MS-DIAL and MzMine can produce a metabolome table of sufficiently high quality if the data are acquired at the same time in the same institute and if the data are analyzed by researchers who are familiar with the background of the analytical conditions used. The difficulty lies in the re-analysis of data acquired by others, including public data registered in MetaboLights and MetabolomicsWorkbench. Metadata and secondary data in public data repositories need to be collected so that metabolomics data can be reanalyzed without special knowledge. Tools to support the interpretation of the metabolome table are also needed.

Recently, the diversity of omics data has increased and become multimodal, including different types of multi-omics data, fragmentation techniques, and spatial omics methods. Therefore, it is important to develop informatics tools that link metabolomics data with other data. In particular, I focus on lipid biochemistry, but it is not easy to link lipid-related genes and metabolites. I believe that data-driven research will be further accelerated when the environment for data analysis is more established.

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

Metabolomics has a wide range of applications, and metabolomics will continue to be used as an adjunct to any budget proposal. If metabolomics is to play a central role in budget formulation, research of machine learning in metabolomics data and of understanding spatiotemporal metabolisms are expected to be of high importance.

What role can metabolomics standards play?

My thoughts on metabolomics standardization are described above. Metabolomics research, which aims to understand the metabolic systems, is mainly performed using mass spectrometry (MS). Recently, the amount of MS data in public repositories has continued to grow (>100 TB), making it imperative to accelerate not only the data management but also the re-analysis and knowledge generation process. As metabolomics standardization and metadata development progress, it will be possible to establish a smooth infrastructure for MS data re-analysis and create an informatics environment for hypothesis generation and knowledge expansion that cannot be achieved by humans. Specifically, (1) the construction of a novel molecular annotation infrastructure using MS spectral machine learning, (2) the construction of a tissue/cell type estimation infrastructure using metabolome machine learning, and (3) the construction of an analysis environment that integrates metabolic imaging data and spatial transcriptome data using these platforms. I believe that this will enable the construction of an analysis environment that integrates metabolic imaging data and spatial transcriptome data. If this can be achieved, it will be possible, for example, to visualize metabolite/gene expression information in biological tissues at the cellular level, which will advance the understanding of metabolite diversity and its regulatory mechanisms. It would also be possible to create a database encompassing the spatio-temporal dynamics of metabolomes (metabolic cartography) by re-analyzing public data. Such knowledge of metabolome information will undoubtedly accelerate data-driven metabolic research.

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

After I moved from RIKEN to a university, my research activities are now led by students in my lab (Figure 3). I strongly believe that it is important to have a solution to accelerate program development and data science. However, in order to sustain these activities and make them more attractive, it is currently essential to have good informatics staff. Of course, there will be efforts to get budgets, but it seems to me that the speed of development would be much more advanced if students were involved in research and development. For this to happen, the cost of program development needs to be lowered,

and I have great respect for OpenMS and MZMine for their early efforts to address this issue. In the last 1-2 years MS-DIAL has become much more open source and the number of developers has increased. My current goal is to make as many students and researchers as possible aware of the interest in metabolomics research and to promote research activities more than when I was at RIKEN by sharing the joy of discovering new facts in the life sciences.

Figure 3: *Dr. Tsugawa and his students from his lab group.*

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The Metabolomist Podcast

THE METABOLOMIST

New episode
Vitamins & metabolic syndrome

> One thing that's exciting about being young in this young field is, we are seeing our mentors be innovators. And that's something we get to carry forward to the next students that we mentor.
>
> **- Haley Chatelaine**

LISTEN NOW

Recent Publications

Reviews:

- Microbial single-cell mass spectrometry: status, challenges, and prospects
- Saliva Metabolomic Profile in Dental Medicine Research: A Narrative Review (Open access)
- Targeting the Gut Microbiota in Kidney Disease: The Future in Renal Nutrition and Metabolism
- Untargeted metabolomic approaches in food authenticity: A review that showcases biomarkers

Articles:

- An integrated deep learning framework for the interpretation of untargeted metabolomics data
- Environmental organic contaminant body burdens and GC-MS based untargeted metabolomics in mediterranean mussels from Port Phillip Bay, Australia
- Flash entropy search to query all mass spectral libraries in real time
- High-throughput MALDI-MSI metabolite analysis of plant tissue microarrays (Open access)
- Integrated analysis of proteomics, epigenomics and metabolomics data revealed divergent pathway activation patterns in the recent versus chronic post-traumatic stress disorder (Open access)
- Integrative metabolomics differentiate coronary artery disease, peripheral artery disease, and venous thromboembolism risks (Open access)

- Lipid metabolic links between serum pyrethroid levels and the risk of incident type 2 diabetes: A mediation study in the prospective design
- Maternal consumption of l-malic acid enriched diets improves antioxidant capacity and glucose metabolism in offspring by regulating the gut microbiota (Open access)
- Metabolomic profiles of obesity and subgingival microbiome in periodontally healthy individuals: A cross-sectional study (Open access)
- Multiomics analysis reveals the molecular basis for increased body weight in silkworms (Bombyx mori) exposed to environmental concentrations of polystyrene micro- and nanoplastics (Open access)
- Multiomics analysis to explore blood metabolite biomarkers in an Alzheimer's Disease Neuroimaging Initiative cohort
- Per- and polyfluoroalkyl substances (PFAS) and thyroid hormone measurements in dried blood spots and neonatal characteristics: a pilot study (Open access)
- Soil metabolomics: A powerful tool for predicting and specifying pesticide sorption
- Towards a Precise NMR Quantification of Acute Phase Inflammation Proteins from Human Serum(Open access)
- Towards a Rosetta stone for metabolomics: recommendations to overcome inconsistent metabolite nomenclature

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Metabolomics Events

Bits & Bites # 07: Introduction to Metaboanalyst

November 2, 2023

Venue: Online

Learn More Here

This 9-part short course series will feature in-depth topics in untargeted metabolomics. Each short course can be taken individually or you can select multiple Bites. You will gain a deeper insight into current software, methods, and pitfalls. Each session starts promptly at 9 a.m. (Pacific Time) and will take approximately 4 hours. The courses will be conducted in highly interactive manner, with use of freely available software and databases. The tuition is $175.

This 7th course is taught by Dr. Jeff Xia from McGill University, and basic knowledge of computer skills and no prior coding experience or software is needed. This short course will cover how to use MetaboAnalyst 5.0, a comprehensive platform dedicated to metabolomics data analysis. There will be a brief overview of data input, processing, and general workflow to perform PCA/PLS-DA/OPLS-DA analysis in MetaboAnalyst. More importantly, this course will cover how to use different functional analysis methods such as Enrichment Analysis, Pathway Analysis, Joint Pathway Analysis, and Network Analysis. Lastly, participants will also learn how to perform biomarker analysis and statistical analysis with complex metadata.

Bits & Bites # 08: Tips & Tricks of GC-MS in Metabolomics

November 16, 2023

Venue: Online

Learn More Here

This 8th course is taught by Dr. Oliver Fiehn from UC Davis. Basic knowledge of computer skills, but no coding experience is needed. The required software is MS-DIAL for Windows. Versions of the tool to be used will be announced closer to the course date. The tuition is $175.

Short description of the course: While LC-MS is all the hype in today's portfolio of metabolomics assays, ranges of small molecules are difficult to impossible to screen in this manner. Volatile compounds in breath, urine, or plant analyses can best be analyzed by GC-MS. Additionally, swaths of primary metabolic intermediates ranging from glycolysis and pentose phosphates to TCA compounds, sugars, and small microbial metabolites are readily and cost-efficiently

analyzed by GC-MS. In this short course, we discuss the fundamentals of GC-MS, tips for best practices, and aspects of instrumentation, and demonstrate data processing and use of databases. Participants will also learn the current challenges, trends, and developments of GC-MS-based metabolomics.

IV LAMPS meeting | American Metabolomic Profiling Society

November 2 – 4, 2023

Venue: Cartagena, Colombia

Learn More Here

IV LAMPS meeting will be held in Cartagena, Colombia Nov 2-4, 2022 at the Universidad de los Andes - Sede Caribe located in the Serena del Mar urbanization. This is the first time that the LAMPS meeting is held in Colombia and the first face-to-face meeting after two years of postponing the meeting due to the COVID-19 pandemic. The conference will cover 5 main areas:

- Health & nutrition
- Natural product screening & identification
- Experimental design & data acquisition
- Software & data analysis
- Metabolite identification

Registration is **closed**.

Clinical & Translational Omics Symposium

November 4 – 5, 2023

Venue: Protaras, Cyprus

Learn More Here

Dive into cutting-edge research in Proteomics, Metabolomics, Lipidomics, Bioinformatics & AI, led by experts John Yates III and Jennifer Van Eyk.

List of speakers and chairs

- Albert Sickmann, ISAS, Germany
- Alina Petre, Al.I.Cuza University of Iasi, TRANSCEND at IRO Iasi, Romania
- Cecilia Lindskoog, University of Gothenburg, Sweden
- Christoph Borchers, McGill, Canada
- David Fenyo, New York University School of Medicine
- Eugene Nikolaev, Skoltech, Russia

- George Spyrou, The Cyprus Institute of Neurology & Genetics, Cyprus
- Gunnar Dittmar, Luxembourg Institute of Health, Luxembourg
- Ian Lewis, University of Calgary, Canada
- Jack Wood, University College London, United Kingdom
- Jenya Petrotchenko, McGill, Canada
- Jennifer Geddes-McAlister, University of Guelph, Canada
- Jennifer van Eyk, Cedars-Sinai, USA
- Jesper Olsen, University of Kopenhagen, Denmark
- Joerg Hanrieder, University of Gothenburg, Sweden
- John Yates III, Scripps Institute San Diego, USA
- Konstantinos Makris, Cyprus University of Technology, Cyprus
- Lukasz Jaremko, KAUST, Saudi-Arabia
- Margret Thorsteinsdottir, University of Iceland, Iceland
- Mariusz Jaremko, KAUST, Saudi-Arabia
- Michael O. Glocker, Proteome Center Rostock, Germany
- Nick Shulman, Skyline, USA
- Nicolai Bache, Evosep, Denmark
- Nelson Soares, Sharjah University, UAE
- Oliver Pötz, SIGNATOPE, Germany
- Petr Novak, Czech Academy of Science, Czech Republic
- Rene Zahedi, University of Manitoba, Canada
- Stefan Tenzer Medical University Mainz, Germany
- Wendy Heywood, University College London
- Yassene Mohammed, LUMC, Netherlands

Check out the conference website for program updates.

- Click here for early-bird registration and abstract submission

14th European Nutrition Conference (ENC) FENS 2023

November 17 – 25, 2023

Venue: Belgrade, Serbia

Learn More Here

The 14th European Nutrition Conference will be held in Belgrade, the capital city of Serbia. The theme of the conference is “Food, Nutrition, and Health: Translating science into practice”. Around this theme, the conference will deliver a high-quality program, featuring international speakers across plenary sessions and symposia. Other features of the program will be discussions and debates, industry symposia, panel sessions, and networking opportunities including several specifically catering to early career researchers.

- Late registration is **till November 10, 2023**

Bits & Bites # 09: Metabolomics for Epidemiologists *New course*

December 7, 2023

Venue: Online

Learn More Here

This last, 9th course (for 2023) is taught by Dr. Oliver Fiehn from UC Davis, and no prior knowledge or software is required. The tuition is $175.

Short description of the course: In this comprehensive course, delve into the pivotal role of metabolomic data in modern epidemiology. Epidemiologists increasingly use metabolomic data in large human cohort studies that focus on public health problems and risk factor analyses. Classically, only a few variables were used in epidemiological analyses which were then stratified by multiple adjustments to find robust associations with phenotypes. Now, GWAS analyses have led the way for metabolite-wide association studies. How robust are metabolite data? What are the best normalization strategies? How should we deal with missing data, QC pools, and blanks? How can different studies be combined to increase power? Which identifiers could be used, and what is good coverage for metabolomic studies? These questions will be discussed in this short course to provide an overview of metabolomics including realistic goals and considerations for study designs, and metabolite coverage from commercial providers versus core facilities.

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

December 4 – 8, 2023

Venue: Online

Learn More Here

This 5 day course provides a comprehensive overview of data analysis for metabolic profiling studies focussing on data from NMR spectroscopy and Liquid Chromatography-Mass Spectrometry. It combines lectures and tutorial sessions using open source software to ensure a thorough understanding of the theory and practical applications. To fully benefit from this course, attendees will ideally have a basic knowledge of analytic chemistry techniques.

The deadline for applying is **November 24.**

For more information and to register, click here.

MANA SODAMeet

December 12, 2023

Venue: Online

Learn More Here

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.

World Critical Care and Anesthesiology Conference 2024 (WCAC24)

March 09 – 10, 2024

Venue: Bangkok, Thailand

Learn More Here

World Critical Care and Anesthesiology Conference 2024 (WCAC24) is the 6th Edition educational event which is designed to advance knowledge and expertise in critical care and

anesthesiology that rotates between continents and is organized in collaboration with national and international Anesthesiology and Critical Care societies and associations. The conference is targeted to the international Critical Care Medicine community as well as other healthcare professionals involved in multidisciplinary critical care surgical challenges; For every community, there continues to be a need for surgical and medical teams to evaluate and treat severely injured patients. Check out more information at the conference website.

- Abstract Submission Deadline: **November 30, 2023**
- Speaker and Presenter's Registration Deadline: **December 30, 2023**

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

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

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

Metabolomics Jobs

Metabolomics Jobs

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

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

Job Title	Employer	Location	Source
Chemical Biologist/Ecologist	The Monell Chemical Senses Center	Philadelphia, PA, USA	The Monell Chemical Senses Center
ORISE Postdoctoral Fellowship in Pharmacology/Toxicology	National Center for Toxicological Research U.S. Food and Drug Administration	Jefferson, AR, USA	Metabolomics Society
ORISE Postdoctoral Fellowship in Neuroscience/ Neurotoxicology	National Center for Toxicological Research U.S. Food and Drug Administration	Jefferson, AR, USA	Metabolomics Society
Doctoral Candidate Position	Exosomes Lab & Metabolomics Platform, CICbioGUNE	Derio, Basque Country, Spain	Metabolomics Society

Postdoctoral Research Scientist Position in Exposomics	Britz-Mckibbin Lab at McMaster University	Hamilton, ON, Canada	TMIC website
Laboratory Technician	Matterworks	Somerville, MA, USA	Metabolomics Society
Postdoctoral Researcher in Mass Spectrometry Workflows for Unknown Chemicals	Luxembourg Centre for Systems Biomedicine (LCSB)	Luxembourg	Luxembourg Centre for Systems Biomedicine
Postdoctoral Position for Metabolomics Research in Mitochondrial Disorders	Luxembourg Centre for Systems Biomedicine (LCSB)	Luxembourg	Luxembourg Centre for Systems Biomedicine
Post-Doctoral Fellow	Department of Medical Microbiology & Immunology, University of Alberta	Edmonton, AB, Canada	University of Alberta Careers
Operations Assistant	NovaMT and TMIC Li Node at the University of Alberta	Edmonton, Alberta, Canada	Dr. Liang Li (please contact liang.li@ualberta.ca)
Postdoctoral Research Fellow (LC-MS and Data Science for Metabolomics)	The Li Lab and the Li Node of TMIC, University of Alberta	Edmonton, Alberta, Canada	University of Alberta

MetaboNews Feedback Form

As you noticed, we have changed to a new format starting in April 2023. We hope to provide enough useful content to keep you interested and informed and appreciate your comments and feedback on how we can make this newsletter better. Please fill out this quick survey and let us know your thoughts (your answers will be anonymous). It will only take less than one minute with only two mandatory questions

Fill Out Your Survey Here

We carefully considered all feedback to enhance our newsletter and deliver an improved

experience. The issue on the "clipped email" link at the beginning of the newsletter is fixed, now, you are able to navigate to the clipped section and extend the content.

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

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