Mailchimp Template Test - "MetaboNews April 2024 Issue"

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

Tue, Apr 30, 2024 at 5:01 PM

MetaboNews

This month in metabolomics

April, 2024
Vol 14, Issue 4

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

In This Issue

Please click on the hyperlinked Table of Contents to navigate to specific sections

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

METABOLOMICS 2024

OSAKA, JAPAN

JUNE 16-20

Are you ready to join us in Osaka? Lots of announcements and helpful info below, complete your travel plans soon and we'll see you in Japan!

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

Abstract Submission – Poster Deadline May 16

There's still time to present your work! Poster abstracts will continue to be accepted through May 16. Take a moment to review the webpage for abstract guidelines, themes, sub-topics and scoring rubric.

Reminder: when you submit an abstract, you will receive a confirmation e-mail. If you do not receive a confirmation e-mail, your abstract HAS NOT BEEN RECEIVED. Contact us for assistance if needed.

Registration – Save Money Now!

Take advantage of the discounted registration rates, now through May 20. Receive an extra discount by renewing or becoming a member of the Metabolomics Society BEFORE registering for the conference

Career Night – Job Fair and Round Table

Career Night is back in 2024 – always a high-energy, well-attended event!
Sunday evening will include a job fair for participants to learn about available positions and interact in a relaxed setting with potential employers. One-on-one interviews between employers and candidates may also be conducted during the conference.

CALLING EMPLOYERS!

We are welcoming potential employers looking to fill positions in the next year. Both industry and academic employers are encouraged to sign up for a table, including academic employers with postdoctoral position openings.

View the website to sign-up for a table (free of charge!) – tables available on a first-come basis.

As some participants may not be currently seeking new employment, Career Night also provides an interactive round table event for participants to develop rapport and expand their networks to ready themselves for future employment. View the website for the round table discussion topics.

Japan Visa – Do Not Delay

Details for entry into Japan are available on the website. Most attendees will not require a visa, based on your country of residence. If you do need a Visa, you should apply soon.

For all travelers to Japan, you are required to have a passport that is more than 6 months from expiration and has at least 1 blank page

Calling Student Photographers!

There's an opportunity to share your photography skills during the conference and receive travel funds. See the bottom of the Awards Page for details. Deadline to apply is May 1.

Members' Corner

Board of Directors

Dear Society Members,

It's been a reasonably busy month for the Society. This has been especially so for Natasa, who is the lead of our conference committee. At our recent Board of Directors meeting we were happy to learn that the plans for Osaka are very nicely taking shape. This is thanks to Natasa and her team, as well as this year's conference chairs Professor Eiichiro Fukusaki and Associate Professor Sastia Prama Putri, and the Scientific Organizing Committee. The meeting is coming together well and I am very much looking forward to this. I hope your plans for travel are taking shape.

At this BoD meeting, we also discussed and voted on our Metabolomics Society awards.

There were some fantastic scientists who were nominated and many thanks to those of you who may have nominated metabolomic researchers for our three award categories: We will be awarding two Honorary Fellows, one Metabolomics Society Medal, and one President's Award. Of course, there will be no spoilers here and you'll have to wait until Osaka to find out who our very worthy recipients are for 2024.

You've had the positive news, and now to something very annoying. L Some of you may have got an email purporting to be from me asking for financial help. Some just outright asking for money, some in the past asking for Apple vouchers, and the most recent ones claiming I am stuck abroad in the USA, France, Philippines (in fact just insert a random country), or a friend or one of our Board members needs help getting to a funeral (yes really!), or that I or a colleague are stuck in one of the above random countries and need funds for COVID tests. These seem to be occurring reasonably frequently and are evolving in their complexity and sneakiness. Given the rather specific nature of the more recent emails, where Metabolomics Society is mentioned along with current and past members of the Board, I am left assuming that these disgusting perpetrators are using reasonably sophisticated AI algorithms to generate such spam. Please rest assured that I would never reach out to you in an email to ask for help or money, and definitely not for your bank account details. I'd do that in person in Osaka, so please bring along your wallet J.

But seriously, if you get something that seems to be from the President of the Metabolomics Society or one of the Board of Directors, please check the email address carefully – you'll see that it did not arise from any of us. Also, if there are any associated phone numbers please don't ring them. Simply delete the message and get on with the rest of your day.

The one silver lining to these dark clouds is that many old friends and colleagues have reached out to me to check if these are real messages or bogus, and so it has been lovely to have some side discussions with some of you and to catch up.

All the very best.

Roy Goodacre, University of Liverpool, UK

President, Metabolomics Society

Canadian Metabolomics Conference 2024 Wrap-Up

See You Next Year in Montreal!

Special appreciation is due to our sponsors and our media partners for their generous support.

- **Platinum:** Linearis and Agilent Technologies
- **Gold:** Thermo Fisher Scientific, Waters Corporations, Fluidome, UBC Faculty of Science, UBC Department of Chemistry, Genome BC
- **Silver:** MDPI-Metabolites, Metware Biotechnology, Applied Pharmaceutical Innovation, Genome Alberta, LECO
- **Media Partners:** MetaboNews, Metabolomics Society, MANA

We extend our gratitude to our invited speakers for their efforts to join us at the beautiful campus of UBC and share with us their recent research in metabolomics and its integration with other omics via their exceptional presentations.

- **Plenary Speakers:** Dr. James Heath, Dr. Fiona Brinkman, and Dr. Leonard Foster
- **Keynote Speakers:** Dr. Robert Ernst, Dr. Lara Mahal, Dr. Jennifer Geddes-McAlister, Dr. Daina Avizonis, Dr. Susan Murch, Dr. Chris Gill, and Dr. Oliver Fiehn
- **PIs from TMIC:** Dr. Christoph Borchers, Dr. Philip Britz-McKibbin, Dr. David Goodlett, Dr. James Harynuk, Dr. Tao Huan, Dr. Liang Li, Dr. Dajana Vuckovic, Dr. David Wishart, and Dr. Jeff Xia.

We also extend our gratitude to the organizers for their meticulous planning and execution, as well as to the dedicated volunteers who ensured the smooth operation of CanMetCon 2024.

Congratulations to all orals and poster presenters!
Finally, heartfelt thanks to all attendees for their active participation and engagement, without which this event would not have been possible. Together, your collective efforts have made CanMetCon 2024 a resounding success, and we look forward to continuing this journey of collaboration and innovation next year in Montreal.

MetaboART Research Contest -hosted by the EMN

Images can often be more effective than words in highlighting how research in metabolomics has an impact in global society, university, and industry. This is an opportunity to showcase the importance of the different research projects conducted by members of the Metabolomics Society. It can also be an ideal first step in engaging and networking with the members of the community. Click to learn more about the MetaboART Research Contest and submit your entry by May 16!

International Affiliates' Corner

Australia & New Zealand Metabolomics Society (ANZMetSoc)

Visit: https://anzmetabolomics.org/what-we-do

The ANZMetSoc is offering travel grants for the upcoming 2024 Metabolomics Society Conference. Students and Early Career Researchers can apply for one of two travel grants, to support their attendance at the 2024 MetSoc annual conference, in Osaka, Japan. Two $500 AUD grants will be awarded. To be eligible, applicants must:

- Be a current member of ANZ Metabolomics Society
- Have your abstract accepted for the 2024 conference and attend in-person (please apply for this travel grant assuming that your abstract has been accepted)
- Be currently enrolled in full or part-time education (student) OR within 5 years of obtaining highest degree (early career researcher)
- Submit application before the deadline (April 20 2024, midnight AEST)

For more information and to apply follow https://anzmetabolomics.org/2024travelaward

Réseau Français de Métabolomique et Fluxomique (RFMF)

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

16th RFMF Meeting in Saint-Malo, France

This sixteenth edition of the French Speaking Network of Metabolomics and FLuxomics, to be held at the Palais du Grand Large in Saint-Malo (June 4-6, 2024), will once again provide an opportunity for our thriving community to get together and exchange ideas through 5 thematic sessions: health, agrobioscience, environment, sea sciences and methodologic development. It will feature several plenary lectures by internationally renowned researchers, as well as oral presentations, 180-second Flash presentations and poster sessions. As has become customary over the last few meetings, oral presentation slots will also be dedicated to highlighting the work of young researchers in the field. This will also be an opportunity to highlight the winner of the 2024 thesis prize and the new RFMF honorary member appointed in 2024, who will be pleased to present a summary of their research.

We will be honoured by a number of talented speakers, including **Julijana IVANISEVIC** (Head of Metabolomics Platform, Faculty of Biology and Medicine, Univ. of Lausanne), **Oscar YANES** (CIBERDEM-IISPV Metabolomics Platform & Department of Electronic Engineering, Univ. Rovira i Virgili), **Carla ANTONIO** (Forest Research Centre, School of Agriculture Univ. Lisbon (ISA/ULisbon), **François VERHEGGEN** (Chemical and Behavioral Ecology, Gembloux Agro-Bio Tech - Univ. of Liege) and **Soizic PRADO** (Muséum national d'Histoire naturelle, Unité "Molécules de Communication et Adaptation des Microorganismes" UMR 7245 MNHN/CNRS). We hope to see many of you there ;)

Nordic Metabolomics Society

Visit:www.nordicmetsoc.org

Registration for the 4th Meeting of the Nordic Metabolomics Society is open and details can be found on: https://nmetc2024.fi/.

On behalf of the local organising 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, to 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 showcase your recent metabolomics research.

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

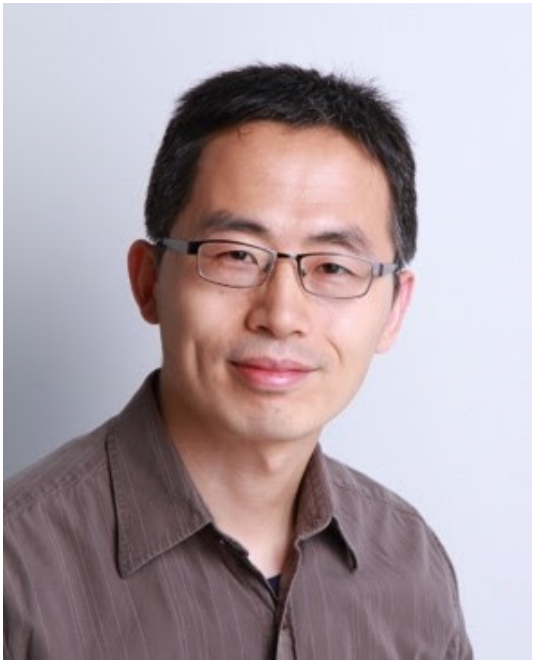
On behalf of the organising committee,

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

Back to top

MetaboInterview

Jianguo (Jeff) Xia



Associate Professor
Canada Research Chair (Tier 2)
Bioinformatics and Big Data Analytics
Institute of Parasitology and Animal Science (joint appointment),
Faculty of Agricultural and Environmental Sciences, McGill University

Xia Lab
Google Scholar

Biography

Dr. Xia is an Associate Professor and Canada Research Chair (bioinformatics and big data analytics) at McGill University, Quebec Canada. His research explores innovative and practical ways to address the current challenges in big data analytics arising from biomedical and environmental research, focusing on metabolomics, transcriptomics, microbiomics and multi-omics integration. His group is actively developing new-generation computational framework integrating cloud computing, machine learning and visual analytics to enable intuitive and high-throughput data analysis. To date, Dr. Xia has authored >100 journal publications and 8 book chapters. He is the 2019 McGill Principal's Prize for Outstanding Emerging Researchers. Since 2019, he has been ranked as Global Highly Cited Researchers (citations: >39,000, H-index: 53) by the Web of Science.

How did you get involved in metabolomics?

I came from a medical background. I am naturally interested in various enabling technologies that have the potential to transform health and disease. In my undergraduate studies, I was fascinated by the Human Genome Project, ENCODE, and their underlying technologies (i.e. sequencing, microarray, etc.) – they were such achievements by leveraging various technologies, and engineering to address big challenges. During my PhD (supervisor: David Wishart, University of Alberta), I was fortunate to be involved in the ongoing Human Metabolome Project with the aim of developing a comprehensive reference database(i.e. HMDB) for the human metabolome. After the initial excitement, I soon realized that it was challenging to directly carve out a

PhD project from such a large, already well-shaped project. I need to work on something complementary.

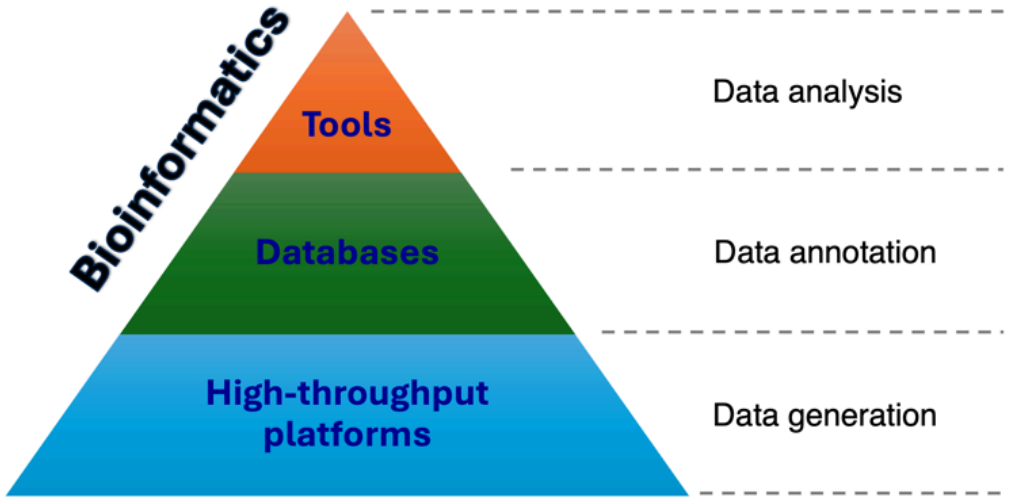


Figure 1: Three Pillars of Omics

For any omics field to "fly" – there must be three key components (Figure 1): high-throughput technologies, reference databases, and bioinformatics tools. The first component is related to instrumentation and is usually tackled by industries; the second component defines the reference framework for a given omics field (i.e. HMDB); the third component varies a lot and is friendly for projects of any size. Clearly, I should consider the category #3 for my PhD project.

In the early stage of metabolomics, there were three prominent bioinformatics gaps: 1) high-throughput, automated compound identification; 2) statistical analysis of data from the metabolomics studies; and 3) functional interpretation. So, I started to tackle these challenges one by one with references to the upstream omics. For the 1st challenge, examples include BLAST for genomics or Macot for proteomics. Can we do something similarly to search the metabolome? This turned out to be quite hard as metabolites are small and their spectra fingerprints do not contain enough information to allow them to be uniquely identified in the database. My first bioinformatics project was to see if we could use 2D NMR for compound identification. I wrote my first software, called MetaboMiner, to perform semi-automated annotation for 2D NMR spectra. This was kind of okay but not at the level of what I would hope it could achieve (i.e. highly sensitive and fully automated). I then started to work on the other two challenges. At that time, the open-source movement became very popular in bioinformatics, especially in the R community (i.e. the Bioconductor project) for gene expression data analysis. I taught myself R and started to use it to perform data analysis and report generations for our collaborators. It soon became clear that data analysis is an open-ended, iterative process, highly

dependent on the researcher and the data - the best way is to let researchers themselves to analyze their own data. This requires a friendly, yet flexible user interface to achieve this. I was very much inspired by the GenePattern and GSEA tools, both developed by the Broad Institute for gene expression profiling and interpretation, respectively. They feature a very intuitive user interface but require local installation (at that time) which is a common barrier for many users. Can we do something similar but through a web interface? I taught myself web technologies and developed MetaboAnalyst for the 2nd challenge (statistical data analysis), and MSEA (metabolite set enrichment analysis) & MetPA (metabolomic pathway analysis) for the 3rd challenge.

After completed my PhD studies, I decided to pursue a postdoctoral position under the supervision of Bob Hancock at UBC, focusing on RNAseq. This choice was driven by my desire to immerse myself in the ongoing revolution facilitated by next-generation sequencing technologies, complementing the research I conducted during my PhD. For ease of maintenance, I merged the web-based tools into MetaboAnalyst, and concluded the first chapter of my encounter with metabolomics.

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

After my postdoc, I started my own lab at McGill in 2015. It was really exciting and also scary to become independent. I could now revisit some of the challenges I did not do well or explore totally new directions.

As I mentioned, my first attempt at automated compound identification did not reach the level I expected. One important reason is the lack of sensitivity related to the NMR technology. Can I solve the issue if I use a high-resolution MS? I acquired an LC-MS Q-Exactive and collected my own data to study host-microbiome interaction using a C. elegans model. Can I use the MetaboAnalyst platform to analyze LC-MS spectra to understand the intricacies of host-microbiome interaction?

It takes me another 10 years to be able answer these questions with a confident "yes!". It is quite a journey. We just published "*MetaboAnalyst 6.0: towards a unified platform for metabolomics data processing, analysis and interpretation*". As the title suggests, we think the three questions (compound identification, statistical analysis, and functional interpretation) are largely solved for LC-MS-based metabolomics. The figure below delineates the roadmap of different versions of MetaboAnalyst over the past decades.

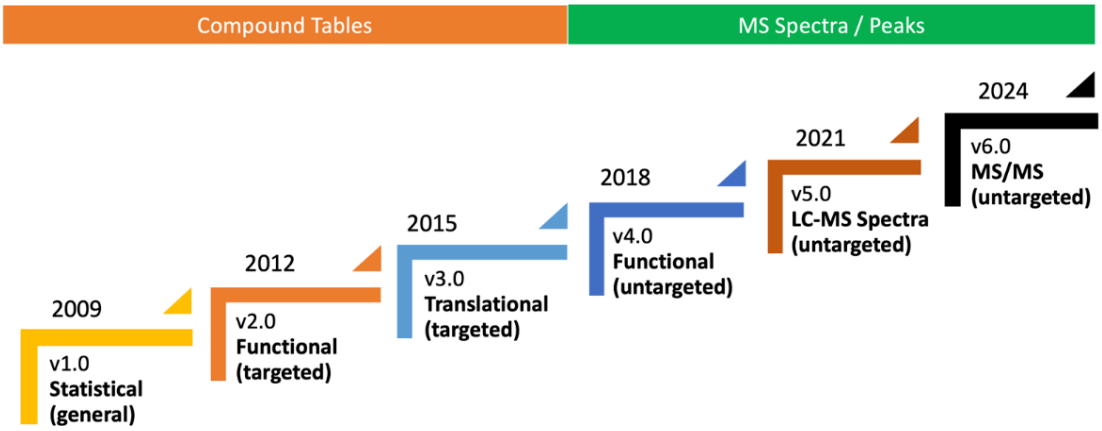


Figure 2: MetaboAnalyst Roadmap

Here I would like to share one fundamental concept, “contextualized data analysis”, which we all use subconsciously in our everyday decision-making, but rarely in data analysis explicitely. The concept is quite useful in omics data analysis. This is because omics technologies measure a lot of things simultaneously – although we may focus on one particular feature (a peak or a metabolite) at a time, the other measured space provides the context. We can leverage this information (as well as other relevant knowledge) to constrain the search space to reach the most likely answers among many possible candidates or scenarios.

For instance, LC-MS metabolomics data typically contain ~10,000 peaks from common biofluids. Many of them cannot be uniquely assigned to a compound when searched independently. However, when we focus on their collective behaviors within the context of our known metabolic pathways or biochemical reactions, the functions can be reliably detected. From the functions, we assign the most likely IDs to peaks. For more details, see mummichog, NetID, and our recent benchmark study. The concept of contextualized analysis has been extensively used in our visual analytics (i.e. the current view defines the context) and functional interpretation. This 6.0 version leveragesMS2 spectra (another contextual information) to further improve functional analysis and compound identification.

The contextual information is what has been captured by the embedding technologies which largely enable the current generative AI. These large language models can accurately understand our natural languages despite their subtleties and ambiguities. Explicitly using an embedding technique for compound identification could be a promising approach.

What is happening in your country in terms of metabolomics?

I am currently a node leader in TMIC, my team primarily works on multi-omics and untargeted metabolomics with applications to microbiomics, exposomics, and foodomics. There are so many intriguing scientific questions to answer and many technical challenges to solve. This is such an exciting field to work on.

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

I would say “integrative” – our metabolome(s) act as interfaces or hubs for many different things – genetics, diet, microbiome, etc. Studying different metabolome(s) will give information on ourselves and our surroundings as well as their interactions.

What do you see as the greatest barriers for metabolomics?

The integrative nature brings its own set of challenges – the instrumentation needs to be integrative (i.e. using multiple instruments to achieve comprehensive coverage) and understanding needs to be integrative (i.e. to adopt multi-omics to understand the full picture). With the availability of many omics centers such as TMIC, the instrumentation challenge has been largely addressed. I would say the key barrier to metabolomics is related to training and better bioinformatics tools to support data understanding and translational applications (will be on that later).

How do you see your work in metabolomics being applied today or in the future? What improvements, technological or otherwise, need to take place for metabolomics to really take off?

The current AI revolution is very exciting, with huge potential to reshape our current research landscape, especially for data analytics. To me, it is very clear that multi-disciplinary team, multi-omics and multi-modality approaches to study health and disease will become the norm in the near future. We are moving from developing infrastructure (early-phase) and conducting large-scale projects for data collection (mid-phase) towards translational applications. Metabolomics will be an integral part of this endeavor. The data collection will become easier and routine for most labs. The future success depends on how to integrate these data and omics technologies to improve health, environment, and agriculture.

In this regard, bioinformatics and more generally, data science will play bigger roles in translating omics data into actionable insights. I firmly believe that the true value of bioinformatics tools is by empowering researchers, clinicians, and policymakers to make informed decisions based on their data. However, this is not straightforward as every researcher is different (background, training, and thought process), and every data is

different (study design, analysis context, and data characteristics), how can we develop tools to effectively meet such needs?

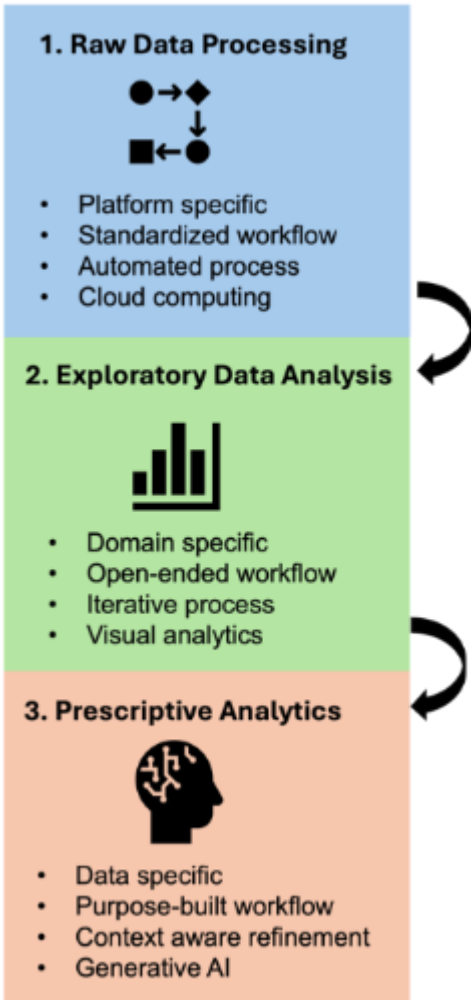


Figure 3: Path to translations

It turns out there are strong patterns in our data analysis. For instance, our omics data analysis can be divided into three stages – raw data processing, exploratory data analysis, and prescriptive analytics. **Figure 3** summarizes the key patterns, characteristics of each stage, and their key enabling technologies. For academic research, we are mainly at the first two stages. The last stage (prescriptive analytics) is vital for translational applications. It is created by “hardening” the most effective workflows derived from the exploratory data analysis. The data will run through the hardened workflow to produce “data-specific” evidence together with other contexts to support decision-making. The only allowed “movable parts” are context-aware refinement according to the current practices of the field of applications.

It is important to emphasize that generative AI technologies, already supporting large context windows and multi-modality data, are poised to play a key role in this process.

What key metabolomics initiatives are you pursuing at your research centre or institute?
How does the future look in terms of funding for metabolomics?
Do you have any other comments that you wish to share about metabolomics?

I started my bioinformatics journey about 15 years ago and soon realized that for most data analysis tasks, many excellent methods and algorithms exist. However, properly using them requires substantial statistical knowledge and computer programming - skills that could take years to master by very few experts (**elite analytics**) and are uninteresting or even distracting to many researchers in life sciences. I felt strongly that omics data analysis should be unintimidating, pleasant, and inspiring to the majority who design their experiments and generate their own data.

The web and cloud technologies have played major roles in making data analytics accessible to a broader audience. Leveraging these technologies, we have implemented a series of tools integrating visualization and statistics (**visual analytics**) to lower the barriers to omics data analysis. These tools have been used by ~1 million researchers worldwide.

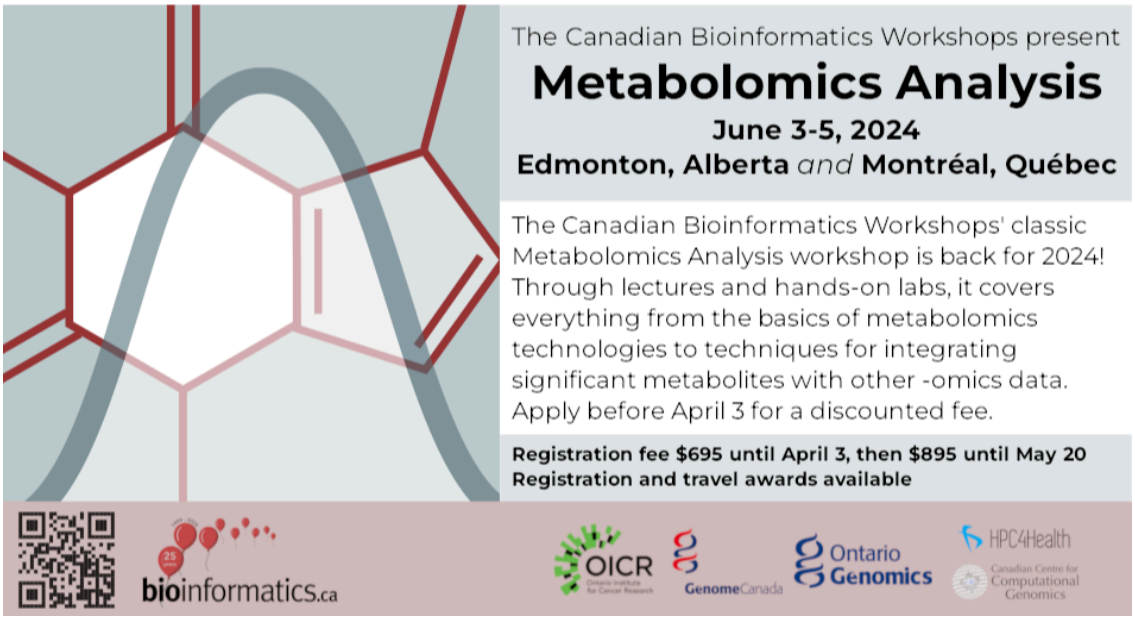
We are at the dawn of a revolution in data analytics. The generative AI technologies allow us to literally chat with our data (**conversational analytics**). An AI assistant, grounded on our omics data analysis tool suites, can recommend workflows, generate reports, and help interpret the data. Data analysis can be greatly simplified yet more effective.
It is both an honor as well as a huge responsibility to support our user community. To avoid the common pitfalls that have led to the demise of many excellent bioinformatics tools, such as the inherent instability of funding and fluctuations of personnel in academic labs, we have recently embarked on a translational journey to help sustain our platforms by providing trainings, pro tools and enterprise support. We have successfully completed our first Omics Data Science training course (January - March 2024). We are now offering two coming sessions:

- Summer Bootcamp (a week in August, tentatively Aug. 5 - 9)
- Regular Session (every Saturday morning, Sept. - Nov.).

You can find more details at https://www.xialab.ca. Thank you for your trust and support.
Please check here for the pdf file

Jeff's group during the Christmas Party

Back to top



Recent Publications

Reviews:

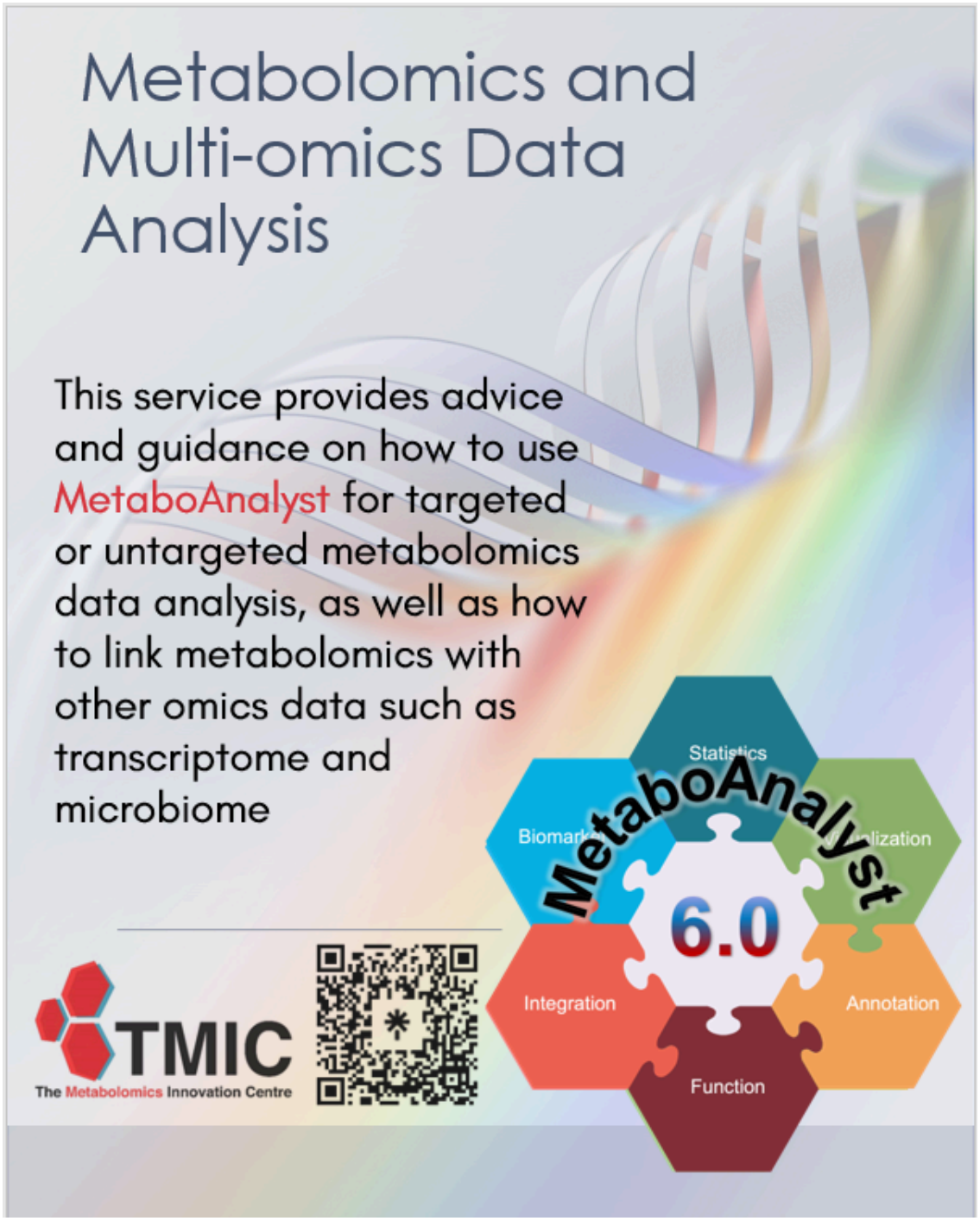
- Lipid Metabolism and Improvement in Oilseed Crops: Recent Advances in Multi-Omics Studies (Open access)

- Molecular aspects of cervical cancer: a pathogenesis update
- Smart selection of soil microbes for resilient and sustainable viticulture (Open access)

Articles:

- Altered serum metabolome as an indicator of paraneoplasia or concomitant cancer in patients with rheumatic disease (Open access)
- Associations of multiple air pollutants with kidney function in normal-weight and obese adults and effect modification by free fatty acids
- Comparison of volatile aroma compounds in commercial surimi and their products from freshwater fish and marine fish and aroma fingerprints establishment based on metabolomics analysis methods
- Comprehensive blood metabolomics profiling of Parkinson's disease reveals coordinated alterations in xanthine metabolism (Open access)
- Deeper insights into the effects of low dietary levels of polychlorinated biphenyls on pig metabolism using gas chromatography-high resolution mass spectrometry metabolomics (Open access)
- High-Throughput Metabolic Pattern Screening Strategy for Early Colorectal and Gastric Cancers Based on Covalent Organic Frameworks-Assisted Laser Desorption/Ionization Mass Spectrometry
- MARS: A Multipurpose Software for Untargeted LC-MS-Based Metabolomics and Exposomics (Open access)
- MetaboAnalyst 6.0: towards a unified platform for metabolomics data processing, analysis and interpretation (Open access)
- Metabolic biomarkers using nuclear magnetic resonance metabolomics assay for the prediction of aging-related disease risk and mortality: a prospective, longitudinal, observational, cohort study based on the UK Biobank
- NMR and MS reveal characteristic metabolome atlas and optimize esophageal squamous cell carcinoma early detection (Open access)
- Plasma metabolic profiles predict future dementia and dementia subtypes: a prospective analysis of 274,160 participants (Open access)
- Plasma metabolomic markers underlying skeletal muscle mitochondrial function relationships with cognition and motor function (Open access)
- Prebiotic proanthocyanidins inhibit bile reflux-induced esophageal adenocarcinoma through reshaping the gut microbiome and esophageal metabolome (Open access)
- Straightforward Creation of Multishell Hollow Hybrids for an Integrated Metabolic Monitoring System in Disease Management
- Soybean steroids improve crop abiotic stress tolerance and increase yield
- Vitamin E biofortification: Maximizing oilseed tocotrienol and total vitamin E tocochromanol production by use of metabolic bypass combinations

Back to top



Metabolomics Events

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

May 9, 2024

Venue: Online

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

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

Check for more details

MANA SODAMeet

May 14, 2024

Venue: Online

The goal of SODA is to provide a community-driven resource of actively-maintained software, test datasets used for software benchmarking, and results produced by software. SODAMeets is a platform where data generators and computational scientists can share their use of software/data. During SODAMeets (every 2 months), two speakers will present on software or data they would like to share with the community, emphasizing how these software/data are

used. Speakers will be requested to fill out a form on our SODA website so that we collect relevant information on these software/data presented.

Join the web seminar

Bits & Bites # 05: Using MS-DIAL to generate accurate comprehensive LC-MS/MS metabolomics datasets

May 23, 2024

Venue: Online

Jake Folz at ETH Zurich is set to teach an intermediate-level course designed for participants who have a basic understanding of LC-MS and the application of MS/MS spectra in metabolite identification. This course will delve into the rigorous demands of metabolomics data processing, especially with large complex datasets (i.e., 1000s of samples, different shipping batches, longitudinal studies). Using hands-on examples, the course provides best practices on how to perform fine-tuned curation of LC-MS/MS data generated through MS-DIAL a freely-available data processing tool for untargeted metabolomics data and other tips for quality assessment and reducing unknown features to ensure accuracy. Versions of MS-DIAL to be used will be announced closer to the course date, and registration details are available below.

Check for more details

2024 Canadian Bioinformatics Workshop series: Metabolomics Analysis

June 3 – 5, 2024

Venue: Edmonton, AB and Montréal, QC, Canada

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

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

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

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

Register for Workshop

II International Conference of the Spanish Society of Metabolomics SESMET 2024

June 3 – 5, 2024

Venue: Seville, Spain – CEU Fernando III University

The conference will cover the most appealing and relevant topics of research in Metabolomics with special focus on Health and Disease, Plant, Food, and Environmental Metabolomics, as well as Microbial Metabolomics. We will delve into Technological Advances including single-cell metabolomics, new matrices, fluxomics, lipidomics, volatolomics, ion mobility, and significant progress in Bioinformatics and Databases. Sessions will explore advances in metabolite identification, multiomics / data integration, databases, metabolic networks, and standardization, among other areas. For more information, including registration details, click below.

Check for more details

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

June 10 – 14, 2024

Venue: in-person at London Hammersmith campus, UK

This 5-day course provides a comprehensive overview of data analysis for metabolic profiling studies focusing on data from NMR spectroscopy and Liquid Chromatography-Mass Spectrometry. It combines lectures and tutorial sessions using open-source software to ensure a thorough understanding of the theory and practical applications.

Registration is open and the early bird rate is until **May 17, 2024.** Standard registration is extended until **May 31, 2024.**

MRC-funded bursaries are available to cover the full early bird fee. The deadline for applying for a Bursary **is extended until May 7** (12.00 BST).

Learn more about the course

20th Annual Conference of the Metabolomics Society

Metabolomics 2024

June 16 – 20, 2024

Venue: Osaka, Japan

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

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

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

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

Learn more here

16th Mass Spectrometry School in Biotechnology and Medicine

July 7 – 13, 2024

Venue: Dubrovnik, Croatia

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

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

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

Learn more here

Back to top

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
Experimental Officer in Metabolomics	University of Birmingham	Birmingham, UK	University of Birmingham
Post Doctoral Position in Human Nutrition: Metabolomics-based exploration	The French National Research Institute for Agriculture, Food, and the Environment (INRAE)	France	INRAE
Post Doctoral Fellow in Metabolomics	Michigan State University	East Lansing, MI, USA	Michigan State University
Assistant Professor, Applied Metabolomics	The Ohio State University	Columbus, OH, USA	The Ohio State University
Postdoctoral Fellow – Microsampling devices for lipidomics	Concordia University	Montreal, QC, Canada	The Metabolomics Innovation Centre (TMIC)

Chemical Biologist/Ecologist	The Monell Chemical Senses Center	Philadelphia, PA, USA	The Monell Chemical Senses Center

MetaboNews Feedback Form

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

Fill Out Your Survey Here

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

Back to top