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**[Test] MetaboNews May 2023 Issue**

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Wed, May 24, 2023 at 11:44 AM

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# MetaboNews

## This month in metabolomics

MAY, 2023

Vol 13, Issue 5

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



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## 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](mailto:info@metabolomicssociety.org)

Membership Enquiries

[membership@metabolomicssociety.org](mailto:membership@metabolomicssociety.org)

## Conference Corner



**[Metabolomics 2023 –Niagara Falls, Canada, June 18-22](#)**

The 19th Annual Conference of the Metabolomics Society will be held at the Niagara Falls Convention Centre in Niagara Falls, Canada from June 18-22, 2023. Abstract submissions have now closed, however registrations remain open, so come and join us in Niagara Falls to check out the exceptional scientific program. As one of North America's most popular family vacation destinations, home to important historical sites, charming villages, and award-winning wineries, Niagara Falls and the Niagara region offer an ideal location to host this conference with convenient access to airports in Toronto or Hamilton (Ontario), and Buffalo (New York).

The oral program is now finalized, and we are looking forward to offering 24 sessions covering a wide range of topics in contemporary metabolomics research. These include sessions on *Cancer, Neurological Disorders and Medicinal Cannabis, Cardiovascular and Metabolic Diseases, Microbiome, Diet and Nutrition, Foodomics and Food Security, New Advances in Lipidomics, Plant Metabolomics, Data Processing and Machine Learning, Data Harmonization and Metabolic Networks*, just to name a few. Choosing the oral program among so many high-quality submissions was an exceedingly difficult task, and we would like to thank our Scientific Organizing Committee, the Board, and EMN for their time and contributions to abstract review and selection.

In addition to the impressive contributed oral program, we are delighted to welcome five exciting plenary speakers: **Lorraine Brennan, Marja Lamoree, Gary Patti, Susan Murch** and **Caroline Johnson** plus ten invited keynote speakers: **Sonia Anand, Takeshi Bamba, Anne Bendt, Ian Castro-Gamboa, Subhra Chakraborty, Hennicke Kamp, Rachel Kelly, María Eugenia Monge, Scott Smid, and Justin van der Hooft**. Of course, we did not forget the [evening and social events](#), with returning classics such as EMN Career Night and Job Fair, Welcome Reception, EMN Reception and Conference Dinner. For our North American attendees, MANA will also host a Networking Reception, while all are welcome to WomiX + FeMS Mixer.

At this time, you can also sign-up to attend the [Platinum Sponsor Lunch Presentations](#). Take a moment to see what our partners have in store and secure your spot today!

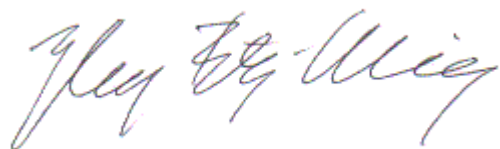
Our conference website includes an overview of the scientific program, details on visa requirements, travel directions to Niagara Falls, and hotel accommodations – most within a short walking distance to the conference centre, the entertainment district of Clifton Hill and the majestic Horseshoe Falls! Please book your hotel reservations as soon as possible using links provided in our conference website as summer is a busy time for tourism in Niagara Falls.

For more information and regular updates please

visit <https://www.metabolomics2023.org/>

We wish you smooth travel to Canada and look forward to welcoming you in Niagara Falls next month!

*Co-chairs of Metabolomics 2023*



Philip Britz-McKibbin  
(McMaster University)



Dajana Vuckovic  
(Concordia University)

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## Members' Corner

### Board of Directors

Dear Society Members,

Niagara Falls is almost upon us :)

The Society's Conference Committee led by Natasa Giallourou, and the conference co-chairs – Phillip Britz-McKibbin and Dajana Vuckovic – along with their International Scientific Committee, have done a great job in getting us ready for Metabolomics 2023. We are very grateful for their excellence and professionalism in putting together a fantastic line-up of speakers and posters.

The full conference program with plenary sessions and three parallel sessions looks enticing and I think it may be hard to decide which of these dual track sessions to attend. We have a packed 5-day meeting starting on Sunday with various workshops (a tradition we started in the early days of the Society's conferences) and ending on Thursday where we shall close out the meeting with our Awards Ceremonies – this will be a wonderful opportunity to celebrate the most influential metabolomics scientists.

For those interested in the running of the Society we have our Town Hall Meeting on

Monday night and here you will find out about what we have been up to since Valencia and what our plans are for the next year. These future plans are not set in stone and up for discussion – we value your input and hope to see many of you there.

Michael Witting, who is leading our Publications Committee, unfortunately won't be with us in Niagara Falls but we will – as we did in Valencia – be discussing plans for our publication strategy. Hopefully you noticed the questionnaire that was sent via e-mail on May 18, please take a moment to complete the short form with your input on a new Society Journal affiliation. The results of the survey will be discussed in Niagara Falls.

Finally, during the meeting we hope to have time to share progress of our scientific task groups and a proforma will be going out to TG chairs soon.

The whole BoD are looking forward to seeing many of you in Canada and we are wishing you safe journeys.

All the very best.

**Roy Goodacre, University of Liverpool, UK**

**President, Metabolomics Society**

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# CanMetCon

Canadian **Metabolomics** Conference



Our 4<sup>th</sup> annual meeting is a symposium on selected topics in **Exposomics** and the latest technologies in **Metabolomics**



Environment and Industrial Settings



Medicine



Clinical Applications



Agriculture/Food /Cannabis

## Exposomics



**Prince of Wales Hotel**  
Niagara-on-the-Lake, ON, Canada



**Thu, Jun 15 - Fri, Jun 16, 2023**  
09:00 AM - 06:00 PM ET



**Registration:**  
C\$150/students, C\$250/general

## Plenary Lectures



**Dr. Joerg Bohlmann**

University of British Columbia  
Combining Metabolome and Transcriptome Profiling for Discovery and Bioengineering in Plant Metabolism: The Novel Anti-Diabetic Metabolite *Montbretin A*

**Dr. Gary Miller**

Columbia University

Exposomics: An Unintended Offspring of Metabolomics



**Dr. Susan Sumner**

University of North Carolina  
Metabolomics and the Exposome in Precision Medicine, Precision Nutrition, and Precision Environmental Health

## Invited Speakers

- Dr. Gerald Batist (McGill)
- Dr. Christoph Borchers (McGill)
- Dr. Philip Britz-McKibbin (McMaster)
- Dr. Jacques Corbeil (Laval)
- Dr. David Goodlett (UVic)
- Dr. James Harynuk (U of A)
- Dr. Tao Huan (UBC)
- Dr. Karl Jobst (MUN)
- Dr. Liang Li (U of A)
- Dr. Dajana Vuckovic (Concordia)
- Dr. Shawn Whitehead (UWO)
- Dr. David Wishart (U of A)
- Dr. Jianguo (Jeff) Xia (McGill)



**TMIC**

The **Metabolomics** Innovation Centre



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[tmic-canada.com](http://tmic-canada.com)

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Dr. Gary W. Miller (Columbia University), Dr. Joerg Bohlmann (University of British Columbia), and Dr. Susan Sumner (University of North Carolina at Chapel Hill) will join us as plenary speakers. Dr. Shawn Whitehead (University of Western Ontario), Dr. Jacques Corbeil (Université Laval), Dr. Karl Jobst (Memorial University of Newfoundland), and Dr. Gerald Batist (McGill University) will each deliver a featured lecture on one of the four topics listed above. TMIC nine node leaders: Dr. Christoph Borchers (McGill Node), Dr. Philip Britz-McKibbin (McMaster Node), Dr. David Goodlett (UVic Node), Dr. James Harynuk (UofA Node), Dr. Tao Huan (UBC Node), Dr. Liang Li (UofA Node), Dr. Dajana Vuckovic (Concordia Node), Dr. David Wishart (UofA A

Node), and Dr. Jianguo (Jeff) Xia (McGill Node) will also present their latest research in metabolomics technologies and exposomics.

In addition to our featured speakers, this conference will host selected speakers from among our registrants, with a few talk spots still available. Ready to share your research? The submission deadline is extended until May 31, 2023, 4 p.m. PST

This conference will complement the larger 19th Annual Metabolomics Society Conference, being held in Niagara Falls only a few days later, giving attendees access to two world-class conferences only days apart. For more information about our conference, please visit our website at [canmetcon.com](https://canmetcon.com).

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## **[Early-career Members Network \(EMN\)](#)**

### **EMN Webinar Series**

The EMN would like to thank once again Prof Dr Alexey Gurevich and Dr Tiago Leão for their insightful and great talks on the challenges of multi-omics, presenting three novel multi-omics bioinformatics tools -- Nerpa, NRPminer, and NPOMix -- for linking gene clusters encoding secondary metabolites to their products. Stay tuned for announcements sent over email and posted on our social media platforms for the upcoming webinar!

### **EMN Workshop**

This year's EMN professional development workshop will focus on Steps Towards Independent Research. As the majority of graduate students envision an academic career, the academic job market is becoming increasingly competitive. Don't miss out on our Professional Career Development Workshop at Metabolomics 2023, where we will discuss personal and professional skills that need to be developed [inside - looking within], as well as identifying and capitalizing on funding lectureship opportunities that are available [outside - looking around], towards increasing your chances of success. [Click here for more details](#).

### **Career Night – Calling Employers!**

The Metabolomics 2023 Career Night is 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. This networking event will allow you to meet with job candidates in Niagara Falls.

Don't miss out on these qualified job candidates! [Check the website](#) to sign up for a table at Career Night. Tables are free of charge, but a limited number are available. Don't delay!

### **MetaboART Research Contest**

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. Learn more about the new [MetaboART Research Contest](#), and submit your entry by May 28!

### **EMN Travel Award**

We are happy to announce the recipients of the 2023 EMN Travel Bursary:

- Jinni Jingya Yan (Sydney Children's Hospitals Network; Westmead, Australia)
- Shuang Zhao (The Metabolomics Innovation Centre; Edmonton, Canada)
- Venus Baghalabadi (Dalhousie University; Nova Scotia, Canada)
- Manish Kumar (Indian Institute of Science Education and Research (IISER); Pune, India)
- Lucien Cayer (University of Manitoba; Manitoba, Canada)
- Monique Ryan (Australian National Phenome Centre at Murdoch University; Western Australia)

We congratulate the awardees and are very excited about the upcoming conference in Niagara Falls!

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## **International Affiliates' Corner**

[\*\*Metabolomics Association of North America \(MANA\)\*\*](#)



Visit: <https://metabolomicsna.org>

MANA is excited to begin a collaboration with the International Lipidomics Society (ILS) and is offering two (2) Early Career Member (ECM) Travel Awards to attend the **8th Lipidomics Forum / 2<sup>nd</sup> ILS conference** and present research that highlights lipidomics. The travel award is a competitive award based on research that displays a high level of distinction, abstract quality and a personal statement. The awards will be selected through a review process by the MANA Awards Committee. Each award includes **\$2000** and a certificate.

Eligibility criteria include:

- MANA member within ten years of a terminal degree
- Must attend and present at iLS
- Conduct lipidomics research in North America

All grant applications must demonstrate the following:

1. Academic achievement
2. Career perspectives
3. Financial need

Conference Information: [The 8th Lipidomics Forum of iLS](#)

Vienna, Austria,

August 27-30, 2023.

**Travel Award Application Deadline: June 2, 2023**

Award information:

[Application Form](#)

[Travel Grant Evaluation Rubric](#)

The MANA ECM Travel Award provides financial support to offset costs of travel or registration fees for professional conferences. This funding enables early career scientists the opportunity to present their research at prestigious conferences and gain valuable networking experience. Please help us support the MANA ECM by encouraging their application.

**[Swiss Metabolomics Society \(SMS\)](#)**

Visit: [www.swiss-metabolomics.ch](http://www.swiss-metabolomics.ch)

## **9<sup>th</sup> Swiss Metabolomics Society Annual Meeting**

**September 15, Zurich, Switzerland**

We are delighted to announce that the 9th Swiss Metabolomics Society Annual Meeting will be held on September 15th in the beautiful city of Zurich, Switzerland. This year's science day will be hosted by Nicola Zamboni in the historic main building of the Eidgenössisch Technische Hochschule Zürich (ETHZ). The theme for this meeting is "Frontiers in Metabolomics", focusing on the latest advancements in analytics, small molecule structure elucidation, omics integration & application, cheminformatics, and computational mass spectrometry. Two renowned plenary speakers are already confirmed! Emma Schymanski and Matej Orešič will be present in Switzerland.

The scientific program will provide young researchers with a unique opportunity to present and discuss their research findings with the metabolomics community. Furthermore, the conference will serve as a platform to facilitate collaboration between international and Swiss metabolomics communities. We look forward to welcoming you to this exciting event! For more conference and registration details, [click here](http://www.swiss-metabolomics.ch).

**ETHzürich**

*Frontiers in Metabolomics*

September 15<sup>th</sup> 2023, ETH Zurich

Host: Prof. Nicola Zamboni  
Rämistrasse 101  
8092 Zurich

Please join us, at ETHZ HG!

Prof. Emma Schymanski  
University of Luxembourg

Prof. Matej Orešič  
Örebro University

Our invited plenary speakers

**Swiss Metabolomics Society:**  
University of Geneva  
University of Basel  
University of Lausanne  
University of Bern  
University of Fribourg  
Swiss Federal Institute of Technology Zurich (ETHZ)  
Functional Genomics Center Zurich (FGCZ)  
**All our members!**

For more exciting programs and registration:  
<https://swiss-metabolomics.ch/annual-meeting/>

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# MetaboNews

**Latest news and insights in metabolomics**



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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.

## Sponsored Spotlight Article

# SpOtlight



## MetwareBio - Pioneer of Widely-Targeted Metabolomics

[Metware Biotechnology Inc](https://www.metwarebio.com/) (MetwareBio) is a metabolomics focused contract research service company that pioneered the Widely-Targeted Metabolomics process and has built a large metabolite database housing data from humans, animals, bacteria, and plants. We are dedicated to providing timely and high quality metabolomics and lipidomics data

for basic research, biomarkers evaluation, food and nutrition research, industrial biotechnology and process development, diagnostics and precision medicine, drug discovery and development, exposomics and microbiome studies.

## 1. Introduction to Widely-Targeted Metabolomics Technology

Metabolomics has a long history of development, with commonly seen approaches such as targeted and untargeted metabolomics. Each of them has its strengths and weaknesses in its throughput, qualitative detection, and quantitative analysis.

Untargeted metabolomics, using DDA (data dependent acquisition) mode from high-resolution mass spectrometers offer precise molecular mass measurement and allows detection of thousands of metabolites in a single run. Targeted metabolomics, using MRM (multiple reaction monitoring) mode allows highly sensitive detection and accurate quantification. These methods are not without limitations and challenges. For untargeted metabolomics, it heavily depends on databases, which contain limited endogenous metabolites from plants or animals, resulting in a limited ability to identify metabolites. Secondly, high-resolution mass spectrometry is less sensitive (by 1-2 orders of magnitude) than low-resolution mass spectrometry, making it difficult to detect low-level metabolites. Lastly, many TOF (Time of Flight) mass spectrometers suffer from dead time problems in their operation mode, leading to inaccurate metabolite quantification. For targeted metabolomics, its disadvantage lies in the limitation of its detection mode, allowing the detection of only a few dozen metabolites in a single run (low throughput), and its dependence on chemical standards for the qualitative identification and quantification of metabolites. These challenges propelled us to develop the Widely-Targeted Metabolomics technology, a process that combines DDA and MRM data acquisition modes based on Q-TOF and QQQ (triple quadrupole) mass spectrometers (see Figure 1). This process was also made possible by the construction of a large, curated database for animals, plants, and humans, allowing for accurate and high-throughput detection of metabolites with ultra-sensitivity and wide coverage.

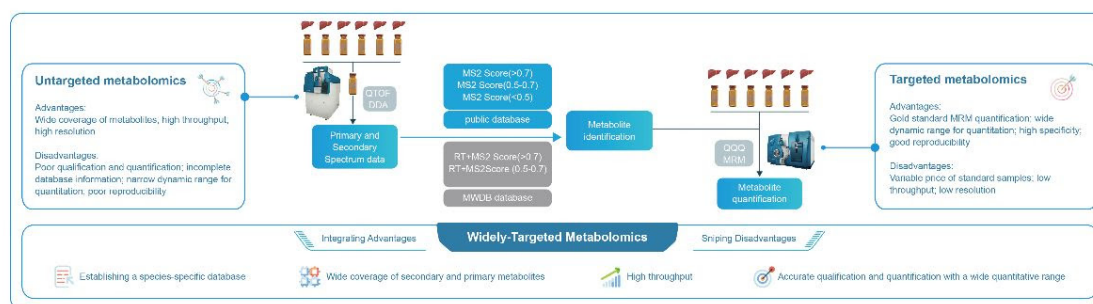


Figure 1. Widely-targeted metabolomics: benefits and workflow

Widely-Targeted Metabolomics was initially developed to create an exclusive database of endogenous metabolites in paddy rice to upgrade the throughput of detected metabolites and assist in studying biological problems<sup>1</sup>. Since then, it has been refined into a metabolomics assay based on a multi-species in-house database. This technique uses the MIM-EPI (Multiple Ion Monitoring–Enhanced Product Ions) mode of a low-resolution mass spectrometer to obtain secondary mass spectra of metabolites. Meanwhile, it refines the parameters required for metabolite identification by utilizing primary and secondary qualitative results from high-resolution mass spectrometry and external sources, such as public databases, standard sample data, and literature. This process culminates in the construction of an MS2 database. The MRM mode is then utilized to optimize collision energy and de-clustering potential for metabolite detection and to select the appropriate Q3 (fragment ion) as the quantitative ion for analysis. By establishing a species-specific endogenous metabolite database, this technique ensures accurate metabolite identification and quantification while greatly improving metabolite detection efficiency.

## **2. Technical features of Widely-Targeted Metabolomics analysis**

Widely-targeted metabolomics is a two-step process. First, untargeted metabolomics using high-resolution mass spectrometers is performed to collect primary and secondary mass spectrometry data from mixed biological samples. These data are compared against databases (public database + in-house library) for high throughput metabolite identification. Then, targeted metabolomics using low-resolution QQQ mass spectrometers in MRM mode is performed to collect mass spectrometry data and metabolite quantity from each sample based on the metabolites detected from the high-resolution mass spectrometer. As a result, this two-step process achieves the following features:

### **a) Accurate annotation**

Widely-targeted metabolomics analysis involves collecting secondary spectra of metabolites in a biological sample using high-resolution mass spectrometry and comparing them with standard spectra in the database. The alignment to the metabolite database is performed using MultiQuant (v 3.0.3) and proprietary software that takes into consideration the retention time (RT), MS1, and MS2 information. The confidence of the alignment is scored using the dot product method.

### **b) Accurate quantification**

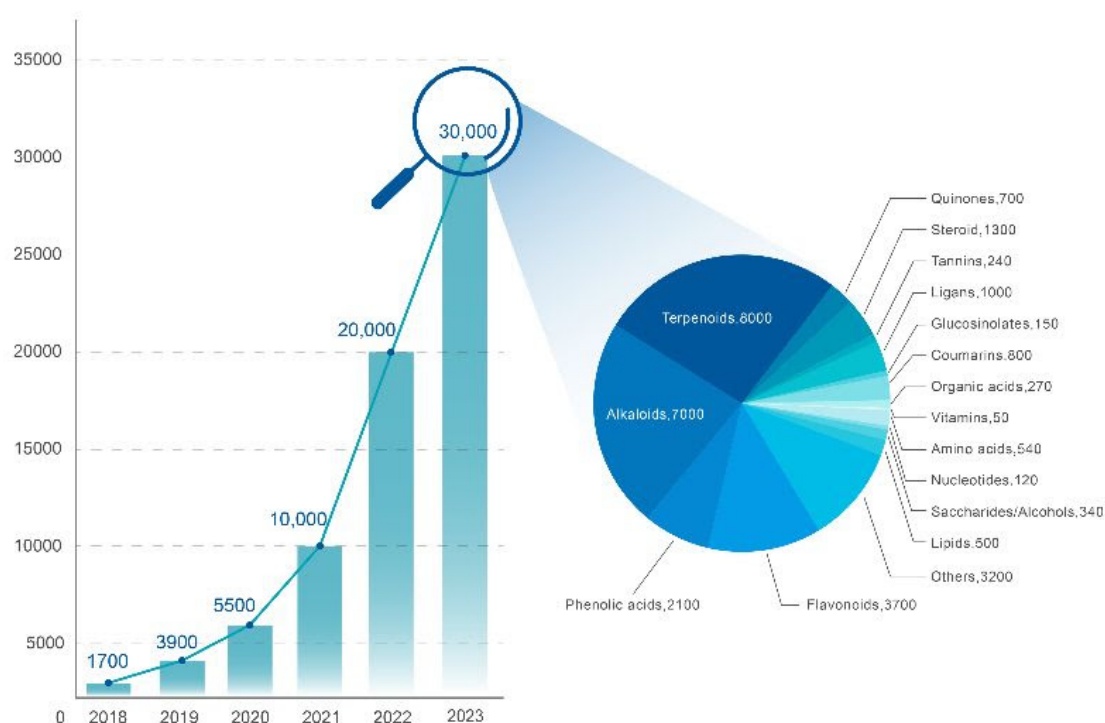
The MRM mode of a QQQ mass spectrometer allows highly specific screening of characteristic ion pairs and reduces the interference from other ions. The MRM mode

also boasts a wide linear dynamic range spanning 4 to 5 orders of magnitude, which facilitates the detection of metabolites across a wide range of concentrations in complex samples. Data processing from MRM scanning is also simplified due to predetermination of selected metabolites.

### c) Large Curated Database

#### Plant database:

Plant metabolites are generally under-represented in the public databases. MetwareBio has constructed a plant metabolite specific database and has been expanding over the last 6 years (Figure 2). It houses over 30,000 plant metabolites to-date that includes primary metabolites (sugars, amino acids, lipids, and nucleotides) and secondary metabolites such as flavonoids, phenolic acids, terpenoids, and alkaloids.



**Figure 2. Growth of MetwareBio's plant metabolite database and the current database size**

#### Human and Animal database:

Our curated database contains over 280,000 metabolites, which includes an in-house database containing over 3,000 metabolites constructed from standards, a curated public database containing over 150,000 metabolites, and an AI predicted structural database containing over 130,000 metabolites. The in-house standard database contains metabolites across 13 different categories as shown in the Table 1 below:



Category	Qty	Representative compounds
Amino acids and their metabolites	600+	Glycine, L-threonine, L-arginine, N-acetyl-L-alanine
Organic acids and their derivatives	400+	3-hydroxybutyric acid, adipic acid, hippuric acid, kynurenine
Nucleotides and their metabolites	200+	Adenine, 5'-Adenine Nucleotide, Guanine, 2'-Deoxycytidine
Carbohydrates and their metabolites	100+	D-glucose, glucosamine, D-fructose 6-phosphate
Lipid	500+	O-acetylcarnitine, $\gamma$ -linolenic acid, lysophosphatidylcholine 22:4
Benzene and its derivatives	500+	Benzoic acid, 3,4-dimethoxyphenylacetic acid, 4-hydroxybenzoic acid
Coenzymes and vitamins	60+	Folic acid, pantothenic acid, vitamin D3
Alcohols, amines	150+	Dopamine, histamine, DL-1-amino-2-propanol
Aldehydes, ketones, esters	120+	Furfural, ethyl butyrate, $\alpha$ -pentyl cinnamaldehyde
Heterocyclic compound	200+	Pyridoxal, biopterin, indole-3-acetic acid
bile acid	40+	Glycocholic acid, deoxycholic acid, tauroolithocholic acid
Hormones and hormone-related substances	100+	Juvenile hormone 3, epinephrine, 3,3'-diiodo-L-thyroxine
Tryptamine, choline, pigment	15+	Serotonin, bilirubin (E-E), urobilin
other	50+	Astaxanthin, hydroxyurea
total		3000+

*Table 1. MetwareBio's In-House Human/Animal-focused Database*

#### d) High reproducibility

The CV values of internal standards across different studies showed that Widely-Targeted Metabolomics is a highly stable assay. Our internal tests showed that quantification of 6 internal standards across thousands of samples remain stable (within 15% CV, see [link for details](#)). Widely-Targeted Metabolomics technology is particularly suited for multi-center, multi-stage biomarker discovery studies. This technology has been applied to identify biomarkers for distinguishing intracranial aneurysm<sup>2</sup>, COVID-19 severity<sup>3</sup>, and follicular development<sup>4</sup>.

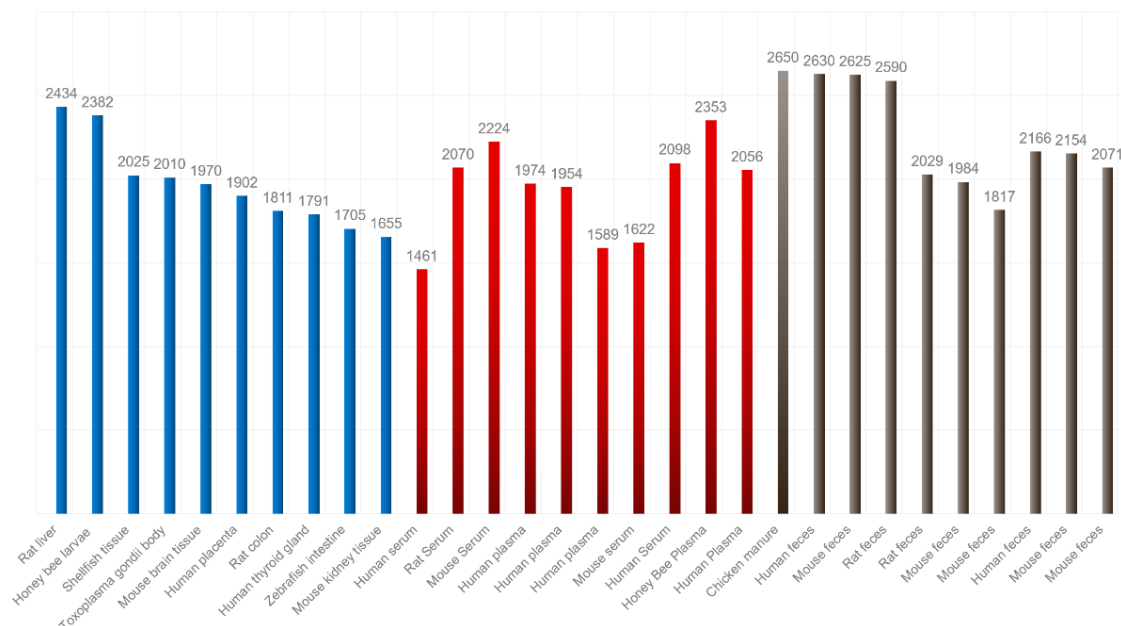
Owing to the large plant metabolite database, Widely-Targeted Metabolomics has also been applied to numerous studies for identifying metabolite biomarkers associated with important agronomic traits, including fruit mass in tomato<sup>5</sup>, plant architecture and height in foxtail millet<sup>6</sup>, and fruit development modulation in mango<sup>7</sup>.

### 3. Widely-Targeted Metabolomics detection results

#### a) Animal samples:

The Widely-Targeted Metabolomics assay detected on average 1800 metabolites in plasma or serum samples, 2000 metabolites in fecal samples, and 1800 metabolites in tissue samples (Figure 3). The range of metabolites was detected, spanning essential categories such as amino acids, organic acids, nucleotides, carbohydrates, fatty acids, glycerophospholipids, and hormones.

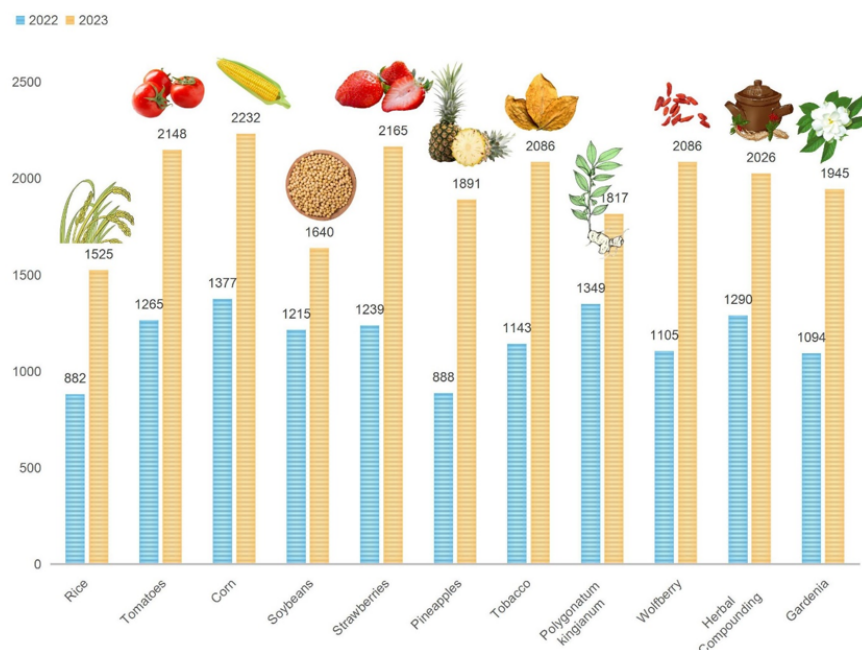




*Figure 3. Number of metabolites detected from various tissues, serum and plasma, and fecal samples*

### b) Plant samples:

Using Widely-Targeted Metabolomics technology, MetwareBio has assayed over 500 plant species. The number of detected metabolites has grown from on average 800 metabolites to 1900 metabolites. Of these, we can distinguish about 700 primary metabolites and 1200 secondary metabolites, which are a diverse set of compounds that confer competitive advantage to the plant's environment<sup>8-10</sup>. Our databases can assist in the development of new plant-based products or therapeutic agents based on these secondary metabolite detections<sup>11,12</sup>.



*Figure 4. A Comparison of Metabolites Detected in 11 Species Over Two Years*

## 4. Metware Cloud



Over the interactions with researchers, clinicians, and breeders, MetwareBio has taken their insights on how they want to visualize metabolomics data and developed a comprehensive tool set for the research community to use. The tools offered in MetwareCloud include individual statistical analytical and visualization tools (e.g. PCA, heatmap, violin plots); it also provides end-to-

end differential analysis. The data input is system agnostic such that you may upload the data for analysis if it adheres to the input format. Any services performed at MetwareBio will have automatic access to MetwareCloud. It is currently free to register and to use by the public as well. More information can be found at <https://cloud.metwarebio.com>.

More details about our assays portfolio (including sample reports) can be found on [our website](#). And by connecting with us on [Twitter](#) and [LinkedIn](#) you will always stay updated on our promotional offers, events where you can meet us and new publications on metabolomics, lipidomics and multiomics.

## 5. References

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# The Metabolomist Podcast



## New episode

Translating metabolomics to the clinics & quality control

” As the metabolomics person, I would always rather have perfect conditions for sample collection. But if your aim is to have a really robust biomarker of use to clinicians, you may want to focus on biomarkers that can survive real-life clinical conditions.

-Jennifer Kirwan

LISTEN NOW



## Recent Publications

### Reviews:

- [Evaluating Software Tools for Lipid Identification from Ion Mobility Spectrometry–Mass Spectrometry Lipidomics Data](#) (Open access)
- [NMR-based metabolomics applied to ecotoxicology with zebrafish \(Danio rerio\) as a prominent model for metabolic profiling and biomarker discovery: Overviewing the most recent approaches](#)
- [PHARMACOGENOMICS: Driving Personalized Medicine](#)
- [Small molecule metabolites: discovery of biomarkers and therapeutic targets](#) (Open access)
- [The need for an integrated multi-OMICs approach in microbiome science in the food system](#) (Open access)

### Articles:

- [Advances and perspectives in chemical isotope labeling-based mass spectrometry methods for metabolome and exposome analysis](#)
- [BUDDY: molecular formula discovery via bottom-up MS/MS interrogation](#)

- [Cardiovascular risk of metabolically healthy obesity in two european populations: Prevention potential from a metabolomic study](#) (Open access)
- [Dynamics of quality attributes, flavor compounds, and microbial communities during multi-driven-levels chili fermentation: Interactions between the metabolome and microbiome](#)
- [Fluorescence-Based Detection of Fatty Acid  \$\beta\$ -Oxidation in Cells and Tissues Using Quinone Methide-Releasing Probes](#)
- [Generation and metabolomic characterization of functional ductal organoids with biliary tree networks in decellularized liver scaffolds](#) (Open access)
- [Genomic atlas of the plasma metabolome prioritizes metabolites implicated in human diseases](#)
- [Identification of plasma metabolites associated with modifiable risk factors and endophenotypes reflecting Alzheimer's disease pathology](#)
- [Insight into the effect of nitrate on AGS granulation: Granular characteristics, microbial community and metabolomics response](#)
- [Metabolomic analysis of maternal mid-gestation plasma and cord blood in autism spectrum disorders](#)
- [Microbiota-derived 3-IAA influences chemotherapy efficacy in pancreatic cancer](#) (Open access)
- [Microplastics promoted cadmium accumulation in maize plants by improving active cadmium and amino acid synthesis](#)
- [Untargeted metabolomics of perfusate and their association with hypothermic machine perfusion and allograft failure](#) (Open access)

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## Metabolomics Events



## Bits & Bites # 04: Using MS-DIAL to generate accurate comprehensive LC-MS/MS metabolomics datasets

**May 25, 2023**

**Venue: Online**

[Learn More Here](#)

This 4th course is taught by Dr. Jacob Folz from ETH Zurich, and participants required to have MS-DIAL for Windows and basic understanding of LC-MS and understanding of how MS/MS spectra are used in metabolite identification.

Short description of the course: Back by popular demand, this short course will focus on how to perform fine-tuned curation of processed LC-MS/MS data generated through MS-DIAL including compound identification, data quality analysis, and unknown feature reduction. Data from rat blood plasma analyzed using LC-MS/MS with MS/MS data collected in a data-dependent manner will be used to generate an example dataset, but the methods and techniques are applicable to many different sample types.

## 20th International GC×GC Symposium

**May 28 – June 1, 2023**

**Venue: Canmore, Alberta, Canada**

[Learn More Here](#)

The symposium brings together researchers, industry experts, and vendors to share knowledge and advancements in the field of GC×GC. Last minute registration is **still available** for the meeting, check for more updates on the symposium website. The scientific program will showcase two GC×GC courses, the GC×GC Awards, and a ton of technical content that covers all of the most recent and cutting-edge developments in GC×GC. Two GC×GC short courses: Introductory GC×GC and Advanced topics in GC×GC run in parallel for about 4 hours. The Introductory Course is intended for those with limited experience with GC×GC or who have never used this technique but are interested in learning more. The Advanced Course is designed for people who are already familiar with GC×GC but want to take their analyses to the next level.



## 71st ASMS Conference on Mass Spectrometry and Allied Topics

**June 4 – 8, 2023**

**Venue: George R. Brown Convention Center (GRB) | Houston, Texas**

[Learn More Here](#)

Advance registration deadline for the conference and short courses for ASMS members: \$300 regular, \$165 students, \$0 emeritus. For non-members: \$550 regular, \$250 students.

All short course registration closes – **May 24, 2023** (may close earlier if capacity limit is met)

Closing event ticket sales – **June 5, 2023**

## MANA SODAMeet

**June 13, 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.



## 4th Annual Canadian Metabolomics Conference (CanMetCon)

**June 15 – 16, 2023**

**Venue: Prince of Wales Hotel | Niagara-on-the-lake, Ontario, Canada**

[Learn More Here](#)

4th Annual Canadian Metabolomics Conference (CanMetCon) will focus on scientific themes in "Exposomics", advancing the understanding of exposures in Medicine, Agriculture/Food/Cannabis, Environment/Industrial Settings, and Clinical Applications. Dr. Gary Miller (Columbia University Mailman), Dr. Joerg Bohlmann (UBC), and Dr. Susan Sumner (UNC at Chapel Hill) will join CanMetCon 2023 as plenary speakers. Dr. Shawn Whitehead (University of Western Ontario), Dr. Jacques Corbeil (Université Laval), Dr. Karl Jobst (Memorial University of Newfoundland), and Dr. Gerald Batist (McGill University) will each deliver a featured lecture on one of the four topics listed above. TMIC's nine node leaders will also present their latest research in metabolomics technologies and exposomics. In addition to our featured speakers, this conference will host selected speakers from among our registrants, with a few talk spots still available. Ready to share your research? The submission deadline is extended until **May 31**. Check out the updated program on the [website](#).

Registration is still open for students is \$150 CAD, and \$250 CAD for all others. All fees are in \$CAD and are subject to applicable taxes and fees.

## 19th Annual Conference of the Metabolomics Society

**June 18 – 22, 2023**

**Venue: Niagara Falls, Ontario, Canada**

[Learn More Here](#)

19th Annual International Conference of the Metabolomics Society will be held on June 18-22, 2023 in downtown Niagara Falls, Canada, at the Niagara Falls Convention Centre. The conference will cover the major scientific themes of: Technology Advances; Computational Metabolomics, Statistics, and Bioinformatics; Metabolomics in Health and Disease; and Metabolomics of Plants, Food, Environment and Microbes. A special theme for this conference will focus on Mental Health, Drug Addiction and Medicinal Cannabis. The scientific program will include plenary and keynote talks, three parallel scientific sessions, interactive poster sessions, sponsor lunches, other networking events and a specially-organized parallel session to promote metabolomics research in industry. To enrich the experience, the conference will offer a welcome reception, vibrant early-career events, a conference dinner and other engaging social activities.

- Late registration is open



Check the [website](#) for topics and requirements.

## Introduction to Nutritional Metabolomics

**June 26 – 30, 2023**

**Venue: Department of Nutrition Exercise and Sports, University of Copenhagen, Denmark**

[Learn More Here](#)

The course will provide a general overview of LC-MS-based untargeted metabolomics from study design to results and will be exemplified by its specific application in nutrition. It will be delivered using a mixture of lectures, hands-on data preparation and analysis, computer-based practical sessions, and discussions. Visits to wet labs and instructions on human sample preparation procedures are included but there is no practical lab work.

## Hands-on Data Analysis for Metabolic Profiling Course

**July 10 – 14, 2023**

**Venue: Imperial College London Hammersmith Campus**

[Learn More Here](#)

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. Early bird registration is open until **June 12**.

## International Summer Sessions in Metabolomics

**August 21 - September 1, 2023**

**Venue: Online**

[Learn More Here](#)

During the summer sessions, participants will engage in both theoretical and practical aspects of metabolomics applications. Utilizing example data sets for training and discussions, attendees will work in small teams to explore various solutions to metabolomic challenges. The course content encompasses study design, sample preparation and compound identification, various metabolomics methodologies, data processing and interpretation, as well as statistical analysis

and data visualization techniques. Additionally, the curriculum covers pathway and network analysis. This course welcomes beginners and advanced users.

## The 8th Lipidomics Forum of iLS

**August 27 - 30, 2023**

**Venue: Vienna, Austria.**

[Learn More Here](#)

A Conference of the International Lipidomics Society and Partners. You will get a chance to learn about the latest lipidomics research from your presentations, posters, and of course from the keynote speakers Frances Platt, Giovanni D'Angelo, Maria Fedorova, Valerie O'Donnell, Peter Meikle, Christoph Thiele, Zoltan Takats, Julijana Ivanisevic, and Andrej Shevchenko. Early bird registration is open until **May 31**.

## Bits & Bites # 05: Identification of unknown compounds in untargeted metabolomics using freely available software

**September 7, 2023**

**Venue: Online**

[Learn More Here](#)

This 5th course is taught by Dr. Arpana Vaniya from UC Davis, and participants required to have basic knowledge of computer skills and no coding experience is needed. The tuition for #5 is \$350 and it takes approximately 8 hours.

Short description of the course: Compound identification is known as the bottleneck in metabolomics. However, there are many approaches one may consider while tackling this challenge (i.e. mass spectral library search, in silico fragmentation tools, or database searching). This short course will provide an overview of the current status of compound ID in metabolomics, participants will learn how to use freely available in silico fragmentation tools MS-FINDER and SIRIUS+CSI: FingerID, web-based tools such as MetFrag and CFM-ID and learn how to use MassBank of North America in NIST MS Search.

## Early Career Members (ECM) Virtual Job Fair

## September 7, 2023

Venue: Online

[Learn More Here](#)

Are you seeking new lab members or exploring new career opportunities? If so, consider attending the Metabolomics Society of North America (MANA) ECM Virtual Job Fair! This event is for employers, recruiters, and job seekers alike, providing a platform to connect with potential candidates or employers from diverse sectors such as academia, industry, or government/nonprofit organizations. Through the virtual Zoom setup, organizers facilitate effortless interactions between employers and prospective candidates, helping you make valuable connections for your career or organization.

## 9th Swiss Metabolomics Society Annual Meeting

September 15, 2023

Venue: Zurich, Switzerland

[Learn More Here](#)

This year's science day will be hosted by Nicola Zamboni in the historic main building of the Eidgenössisch Technische Hochschule Zürich (ETHZ). The theme for this meeting is "Frontiers in Metabolomics", focusing on the latest advancements in analytics, small molecule structure elucidation, omics integration & application, cheminformatics, and computational mass spectrometry. Two renowned plenary speakers are already confirmed! Emma Schymanski and Matej Orešič will be present in Switzerland. The deadline for oral presentation is **June 15** and the poster is **August 15**.

## 5th Annual Metabolomics Society of North America (MANA) Conference

October 23 – 27, 2023

Venue: Columbia, MO, USA

[Learn More Here](#)

The 2023 conference will be held October 23-27, 2023 on the campus of the University of Missouri in Columbia, MO. Professor Lloyd Sumner will chair the meeting and is developing an exciting program that will appeal to many interests in metabolomics. This year, MANA is excited to partner with the International Lipidomics Society (ILS), and the 2023 conference will have dedicated sessions for lipidomics, and an evening workshop with the ILS. Check out the conference website for program updates.

## 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.

- Abstract submission deadline extended to June 10th, 2023
- July 10, 2023: Early bird registration deadline

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## Metabolomics Jobs

### Metabolomics Jobs

If you have a job to post, please email the MetaboNews team at

[metabolomics.innovation@gmail.com](mailto: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
Operations Assistant	NovaMT and TMIC Li Node at the University of Alberta	Edmonton, AB, Canada	Dr. Liang Li (please contact <a href="mailto:liang.li@ualberta.ca">liang.li@ualberta.ca</a> )

Postdoctoral Research Associate-Sumner Lab	Nutrition Research Institute	Kannapolis, North Carolina, US	<a href="#">The University of North Carolina</a>
Research Associate (Computational Metabolomics)	Leibniz Institute of Plant Biochemistry	Helle, Germany	<a href="#">Leibniz Institute of Plant Biochemistry</a>
Postdoctoral Research Associate - Pharmaceutical Sciences	St. Jude Children's Research Hospital	Memphis, Tennessee, USA	<a href="#">Metabolomics Association of North America</a>
Postdoctoral Position in Big Data Analytics for Metabolomics and Exposomics	Du-Lab Research, North Caroline at Charlotte	Charlotte, North Carolina, USA	<a href="#">Du-Lab</a> (please contact <a href="mailto:xiuxia.du@uncc.edu">xiuxia.du@uncc.edu</a> )
Doctoral Candidates	HUMAN – Harmonising and Unifying Blood Metabolomics Analysis Networks	Europe	<a href="#">HUMAN Doctoral Network</a>
Senior Research Associate - Small Molecule and Metabolomics	Corteva	Des Moines, Iowa, USA	<a href="#">Metabolomics Association of North America</a>
Research Technician in Mass Spectrometry	The Wishart Lab and the Wishart Node of TMIC, University of Alberta	Edmonton, Alberta, Canada	<a href="#">University of Alberta</a>
Assistant Professor in Mass Spec and/or Metabolomics	Michigan State University	East Lansing, Michigan, USA	<a href="#">Michigan State University</a>
Postdoctoral Research Fellow	Cincinnati Children's Hospital Medical Center	Cincinnati, OH, USA	<a href="#">ASMS Careers</a> or contact Xueheng Zhao ( <a href="mailto:xueheng.zhao@cchmc.org">xueheng.zhao@cchmc.org</a> )
Postdoctoral position in Microbial Ecology/Metabolomics	The Moran and Edison labs at the University of Georgia	Athens, GA, USA	<a href="#">Center for Chemical Currencies of a Microbial Planet</a>

Mass spectrometry specialist	University of Miami	Miami, FL, USA	<a href="#">Metabolomics Association of North America</a>
Staff Scientist - Raman spectroscopy	Neuro-Oncology Branch, National Cancer Institute, National Institutes of Health	Bethesda, MD, USA	<a href="#">National Cancer Institute</a>
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	<a href="#">University of Alberta</a>
Various Positions	Various	Various (within North America)	<a href="#">Metabolomics Association of North America</a>

## MetaboNews Feedback Form

As you noticed, we change to a new format starting this April 2023 issue. 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](#)

If you have any questions, don't hesitate to contact us at [metabolomics.innovation@gmail.com](mailto:metabolomics.innovation@gmail.com)

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