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# MetaboNews

## This month in metabolomics

February, 2024

Vol 14, Issue 2

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



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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)

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## Conference Corner



Planning is shaping up for the in-person conference in Osaka, at the ATC Hall located right on the bay. Join us in Japan, June 16-20, 2024, for plenary sessions, a busy exhibit hall with industry partners and a huge poster gallery, workshops, and over 25 scientific sessions!

**Website:** [www.metabolomics2024.org](http://www.metabolomics2024.org)

**Hosted by:** The Metabolomics Society

**When:** June 16-20, 2024

#### **Abstract Submission- Deadline March 7 for oral abstracts!**

Abstract submission is now open. Submissions for oral abstracts will be accepted through March 7. 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.

Abstract Info: <https://www.metabolomics2024.org/abstract-submissions>

There are several **Travel Awards** available to support all types of participants. Review the details online before submitting your abstract, you might be eligible!

#### **Conference Registration Open!**

Conference registration is now open. Save money and register online before April 1 to receive the discounted early rate. Members receive an extra discount, so become a member of the Society before registering for the conference for savings!

## **Members' Corner**

## Board of Directors

Dear Society Members,

As a resident in the northern hemisphere, the end of February – early March is my favourite time of the year as the days noticeably start to draw out, the spring blossom initiates its bloom and currently, my snow drops are proudly parading their flowers, with daffodils soon to follow (which as a Welsh man – dw'in Cymro – are very special).

This leap year is very special for the Metabolomics Society as this is our 20<sup>th</sup> year! As someone at its inception, it's quite hard to believe that this international union originated in 2004. If like me, you remember Steve Oliver and Doug Kell's paper being published in *Trends in Biotechnology* in September 1998, you will know that this was the first time the term 'metabolome' was introduced to the scientific literature. It is astounding that a search today in Clarivate's Web of Science returns nearly 85,000 papers when using the search term "metabolome\* (All Fields)". Our field is certainly thriving just like my spring bulbs!

Yet, despite the number of publications approaching 100k, there are still some big challenges our field faces in terms of metabolite annotation and identification, quantification of metabolites, and probably the reason most of us got interested in this field: how one can extract biochemical meaning from these data on small molecules and integrate this with other relevant biological information.

Henry Nix said in 1990\*:

"Data does not equal information; information does not equal knowledge; and, most importantly of all, knowledge does not equal wisdom. We have oceans of data, rivers of information, small puddles of knowledge, and the odd drop of wisdom."

I don't really think with metabolomics that there is much of an issue with data flow (although one can always do with a little more, eh!). The bottleneck we need to address is how to extract wisdom from these data. As metabolomers we have ideas on how to get closer to this wisdom so that we can understand more about our favourite biological system. We can't do this in isolation and the natural diversity in our science has been key to the successes in our field over the last 20 years or so. This is perhaps why as a field we are very welcoming to all people, all research ideas and areas, and long may this growth in our family continue.

Now to more pressing things.

Please note that there are several looming deadlines:

- The first is for the nominations for our Metabolomics Society 2024 Awards which closes on Thursday 29 February 2024. Please get those nominations in for our: Honorary Fellowships, Metabolomics Society Medal, and President Award. Details are currently on our homepage <https://metabolomicssociety.org>) and will be until these nominations close.
- Also closing before 1 March 2024 is the call for interest in hosting our Metabolomics 2026 conference. In 2026 we will be having our annual meeting in the North and South America region. If any of you are interested in hosting our conference, then please visit our homepage for a link to a short Google form.
- The last dates I should tell you about are our deadlines for abstract submission for this year's meeting in Osaka.
  - The Oral Abstract deadline is Thursday 7 March 2024.
  - Poster Abstracts deadline is Thursday 16 May 2024.

All the very best.

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

**President, Metabolomics Society**

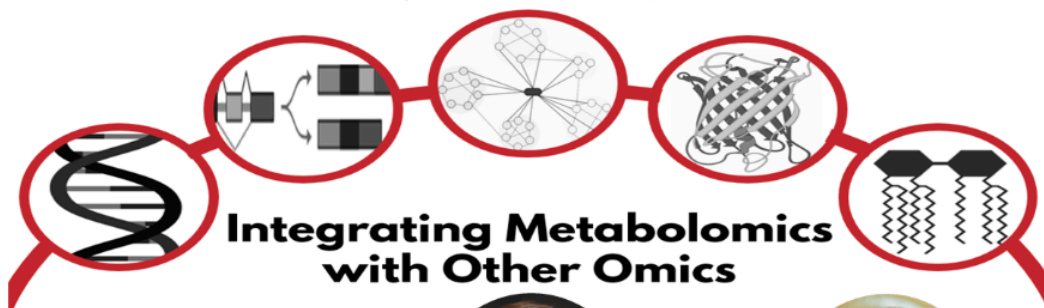
*Where it all started if you need to be reminded:*

Oliver, S. G., Winson, M. K., Kell, D. B. & Baganz, F. (1998). Systematic functional analysis of the yeast genome. *Trends Biotechnol* 16, 373-378. [https://doi.org/10.1016/S0167-7799\(98\)01214-1](https://doi.org/10.1016/S0167-7799(98)01214-1)

\*Nix's Keynote address was to AURISA (Australasian Urban and Regional Information Systems Association Inc.).

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## The 5<sup>th</sup> Canadian Metabolomics Conference 2024



**James Heath**

**Institute of Systems Biology**  
 Integrating Metabolomics into Single  
 Cell Immunophenotyping Toolsets



**Fiona Brinkman**

**Simon Fraser University**  
 Integrating Omics Data to Benefit  
 Communities



**Leonard Foster**

**University of British Columbia**  
 Integrating across 'omes to understand  
 the pathology of acute spinal cord injury

### Invited Speakers:

- Daina Avizonis (McGill University)
- Christoph Borchers (McGill University)
- Philip Britz-McKibbin (McMaster University)
- Robert Ernst (University of Maryland Baltimore)
- Oliver Fiehn (University of California Davis)
- Chris Gill (Vancouver Island University)
- Jennifer Geddes-McAlister (University of Guelph)
- David Goodlett (University of Victoria)
- James Harynuk (University of Alberta)
- Tao Huan (University of British Columbia)
- Liang Li (University of Alberta)
- Lara Mahal (University of Alberta)
- Susan Murch (University of British Columbia)
- Dajana Vuckovic (Concordia University)
- David Wishart (University of Alberta)
- Jeff Xia (McGill University)



**Jack Poole Hall, UBC, Vancouver**



**April 25–26, 2024**



**Registration:**  
**C\$150\*/students C\$250\*/general**  
 \*plus taxes and fees

### Register and Submit Your Abstract Now!

We are accepting abstracts for  
 short talks and posters

Visit us: [canmetcon.com](http://canmetcon.com)



### Act now! One week left for the Early Bird Registration

With just one week remaining, take advantage of the early bird registration for the conference. Don't miss your last chance to secure the discounted rate.

The 5th Annual Canadian Metabolomics Conference (CanMetCon 2024), scheduled for Thursday, 25 April to Friday, 26 April 2024, at the Jack Poole Hall, The University of British Columbia, Vancouver, BC, co-hosted by The Metabolomics Innovation Centre (TMIC) and the UBC Department of Chemistry.

This year's conference is themed "Integrating Metabolomics with Other Omics", featuring

four broad topics in the applications of Biological and Cellular Systems, Omics in Clinical Studies and Biomarker Discovery, Agricultural and Nutritional Applications, and Public Health and the Epigenome.

More information about the program is available [here](#)

Registration is open now! Important dates:

- Early Bird Registration deadline: **February 29, 2024**
- [Abstract Submission](#) Deadline: **March 15, 2024** to be considered for Oral Presentation, **March 22, 2024** for Posters
- Registration Deadline: **March 22, 2024**

Early bird registration fees are **CAD 150** for students and **CAD 250 plus applicable taxes and fees**. Your registration fee includes a welcome reception on April 25, breakfast and lunch on April 25–26, and light refreshments during morning and afternoon coffee breaks. See you in Vancouver!

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

#### **EMN Webinar Series**

EMN Live Webinar Series: 9th session, took place on Thursday, February 15th, at 14:00 UTC, featuring Dr. Maria Fedorova. She is an Associate Professor for the Lipidome Research Center at the University Hospital Carl Gustav Carus and Faculty of Medicine of TU Dresden, Germany. Using innovative mass spectrometry and bioinformatics solutions, her group looks at the lipid quality control machinery at subcellular, cellular, and organismal levels. Prof. Fedorova discussed lipidomics high-throughput LC-MS workflows exploring the diversity and functions of lipids through advanced bioanalytical and computational tools. Look for the recording of the webinar to be posted on the Society website in the Resources section.

#### **EMN Networking Committee**

Registration is now open for the 2024 ECR Virtual Networking Event! This event, co-organized by the Metabolomics Society and the Metabolomics Association of North America (MANA), is scheduled for March 21st at 9:00 AM EST. Join us at <https://bit.ly/ECRNetworking2024>.

#### **EMN Conference Committee**

This year, the EMN is again opening the MetaboArt competition to allow showcasing research projects in metabolomics through creative ideas. We strongly recommend the participation of scientists at any stage of their career as we strongly believe that images can be more effective than words in explaining scientific research. Stay tuned for the

coming opening day in April. The winners of the MetaboART competition will be announced at the EMN reception at the Metabolomics 2024 conference in Osaka.

### **EMN Travel Bursary Committee**

The 2024 EMN Travel Bursary Awards aim to provide support for Early-Career scientists to attend and actively participate in Metabolomics 2024 in Osaka, Japan to promote their professional development. To apply, submit an abstract for the conference and select "Yes" for the EMN Travel Bursary. Complete all application questions that follow. There is not a separate application form, the application is contained within the abstract submission process. Decisions will be communicated to all applicants over email by early May, and winners will be announced on the Metabolomics Society website, social media platforms, and in the MetaboNews newsletter. The application deadline is March 7, 2024 (abstract must also be submitted by March 7).

## **International Affiliates' Corner**

### **Réseau Français de Métabolomique et Fluxomique (RFMF)**

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



### **Workflow4Metabolomics**

Since 2014, the Workflow4Metabolomics core team and RFMF have annually hosted an international "Bring Your Own Data" training session. The recent Workflow4Experimenter 2023 School (W4E2023) occurred from March 20th to 24th at the Institute of Complex Systems in Paris, France. This edition attracted 24 participants from diverse geographical and thematic backgrounds, focusing on metabolomics data processing (LC-MS, GC-MS and NMR).

Throughout the training week, participants engaged with the workflow4metabolomics infrastructure and the Galaxy environment. The 2023 format incorporated feedback from the previous year, featuring remote webinars introducing methodological concepts and tool presentations. The subsequent in-person week allowed hands-on data processing, supported by tutors from reputable French and Belgian laboratories, and a member from Masaryk University (Czech Republic), responsible for the "Spectrometric Data Processing and Analysis" team. This team's tools, dedicated to High-resolution GC-MS data processing, were recently integrated into the W4M instance, enhancing the community's

toolbox.

In 2023, two remote keynote presentations were delivered by Dr. T. Payne (EBI, United Kingdom, for Metabolights) and Dr. N. Poupin (INRAE Toulouse, for Metexplore). The overwhelmingly positive feedback from participants (75% very satisfied, 25% satisfied, and 81% achieving personal objectives) marked the event's success, particularly with the implementation in two sessions.

Looking ahead to 2024, W4E will maintain the 2023 format (webinars + practical sessions) and take place in Grenoble, France. In line with the RFMF philosophy, conviviality and gastronomy were not forgotten.

## **Latin American Metabolic Profiling Society (LAMPS)**

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

We are thrilled to announce our upcoming V Latin American Metabolic Profiling Society (LAMPS) Meeting, scheduled to be held between October 30 and November 1, 2024. This is the most important metabolomics event in our region, and it will be hosted for the first time in Montevideo, Uruguay, at the Auditorio Mario Benedetti located in the Torre de las Telecomunicaciones.

On behalf of both the LAMPS Founding Members and the Scientific Organizing Committee of the Conference, we are excited to welcome you in Montevideo. We look forward to meeting with you all in person to promote the exchange of ideas and future collaborations in the region. News and updates on the conference will be posted on <https://sites.google.com/unesp.br/v-lamps-2024/home>.

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## **Metabolomics Association of North America (MANA)**

Visit: <https://metabolomicsna.org>

Email [mana@metabolomicsna.org](mailto:mana@metabolomicsna.org) | [LinkedIn](#) | X/Twitter [@MetabolomicsANA](#)

Save the date for our 6<sup>th</sup> annual MANA conference! This year, the meeting will take place in Tampa, Florida, USA, October 22-24<sup>th</sup> 2024. Stay tuned for abstract submission and registration details!

Be sure to also check out our [events page](#) for more information on activities from MANA interest groups and committees. Some upcoming activities include our Virtual

Metabolomics Journal Club (contact Karen Howard [khoward@ccrc.uga.edu](mailto:khoward@ccrc.uga.edu) to get involved), and interactive meetings hosted through our [Microbiome](#) and [Software and Data Exchange](#) interest groups.

Other MANA member-led events include the following (see flyers below as well):

- Virtual Networking Event “Navigating International Collaboration and International Mobility” hosted by the MANA Early Career Member Interest Group in collaboration with the Metabolomics Society Early Career Member Network will be held on March 21, 2024 9 am ET/6 am PT, register <https://bit.ly/ECRNetworking2024>
- International Theoretical and Practical Course: "Making Metabolomics Matter: Targeted Approaches for Translational and Precision Medicine". Scholarships for Latin American students/researchers are available and applications must be sent to [yamilelopez@gmail.com](mailto:yamilelopez@gmail.com).

**March 21 / 9 to 10:30 AM EST**

**2024 Early Career Researchers  
Virtual Networking Event**

Theme: *“Navigating International Collaboration and International Mobility”*

**Ewy Mathé**  
National Center for Advancing Translational Sciences (NCATS)  
National Institutes of Health (NIH)  
United States

**Rachel Kelly**  
Harvard Medical School  
Harvard University  
United States

**Stacey Reinke**  
School of Science  
Edith Cowan University  
Australia

**Emma Schymanski**  
Luxembourg Centre for Systems Biomedicine (LCSB)  
University of Luxembourg  
Luxembourg

This event is co-organized by Metabolomics Society (EMN representative: Marvin N. Iman) and Metabolomics Association of North America (ECM representative: Robin Joshi).

Spaces are limited! Register at: [bit.ly/ECRNetworking2024](https://bit.ly/ECRNetworking2024)



Welcome to the International  
Theoretical and Practical Course

# MAKING METABOLOMICS MATTER

Targeted Approaches for Translational and  
Precision Medicine

**JULY 22-26  
2024**



Universidad Nacional Autónoma de México  
(UNAM) Facultad de Química, Ciudad de México



**09:00AM- 6:00PM**



**APPLY NOW**



Contact us:  
[yamilelopez@gmail.com](mailto:yamilelopez@gmail.com)

## PLENARY SPEAKERS



Dr. David Wishart.  
TMIC Wishart Node, University of Alberta



Dr. Yamile López Hernández  
Course Coordinator



Dr. Carlos Alberto Aguilar Salinas  
Instituto Nacional de Ciencias Médicas y Nutrición.



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# MetaboNews

**Latest news and insights in metabolomics**



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## MetabolInterview

### Maria Fedorova



#### **Prof. Dr. Maria Fedorova**

Associate Professor for Lipidome Research

Center of Membrane Biochemistry and Lipid Research

University Hospital and Faculty of Medicine Carl Gustav Carus of TU Dresden

<https://fedorovalab.net/>

### Biography

Maria Fedorova studied Biochemistry at Saint-Petersburg State University, Russia and obtained her PhD at the Faculty of Chemistry and Mineralogy, Leipzig University, Germany. From 2012 she worked as a Group Leader at the Institute of Bioanalytical Chemistry at the University of Leipzig. In 2021 Maria group moved to the Center for Membrane Biochemistry and Lipid Research, TU Dresden. Since 2024, Maria became an Associate Professor in Lipidome Research at University Hospital and Faculty of Medicine Carl Gustav Carus of TU Dresden.

Maria research is focused on understanding the mechanisms behind plasticity, adaptation and maladaptation of natural lipidomes in response to different stressors (metabolic,

redox, etc). Using innovative mass spectrometry and bioinformatics solutions, her group looks at the lipid quality control machinery at subcellular, cellular and organismal levels. Maria also serves as a vice-chair of Pan-European Network in Lipidomics and Epilipidomics (EpiLipidNET), a community of researchers interested in lipid biology and lipidomics technologies, supported by European Cooperation in Science and Technology. Since 2024, together with Maria Eugenia Monge, Maria is a co-chair of the LipidMet task group within the Metabolomics Society.

### How did you get involved in lipidomics?

I am a biochemist by training and my interest in lipidomics was from the beginning triggered by a biological question – how do cells/tissues/organisms adapt to stress? Already within the Master's project, which I did under the supervision of Nadezda Kuleva at St Petersburg State University, I was interested in understanding redox regulation and stress responses in biological systems. When I joined the laboratory of Ralf Hoffmann at the Institute of Bioanalytical Chemistry in Leipzig for the PhD project, I got the opportunity to combine my knowledge in biochemistry and interests in redox biology with advanced bioanalytical methods such as proteomics characterizing protein redox post-translational modifications (oxPTMs).

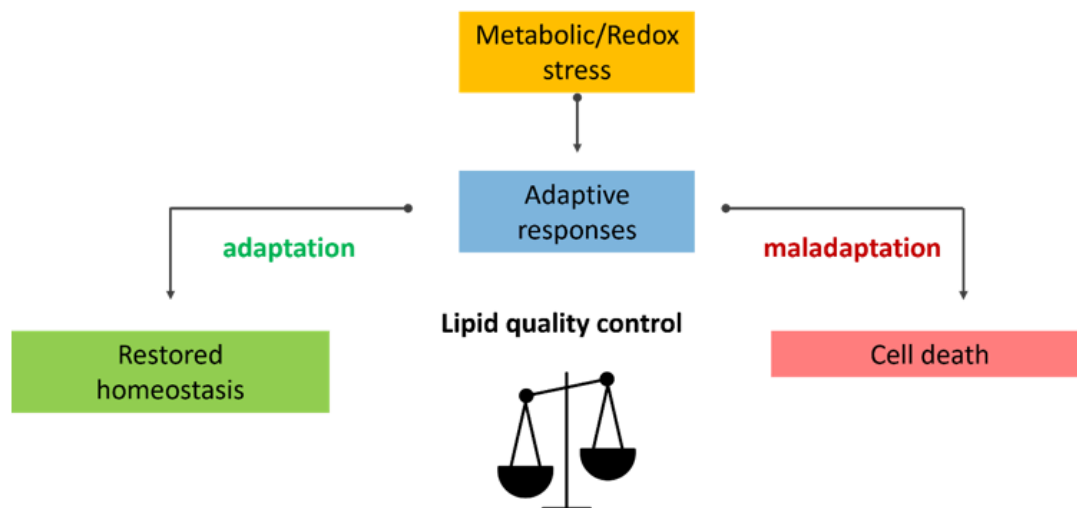
Being fascinated with mass spectrometry as a technique that allows us to measure hundreds of molecular species, characterize their structure (at least to a certain extent), and (relatively) quantify the response, I moved on from proteins to lipids. Why? The choice was governed by the same redox biology questions. One type of oxPTMs are adducts between nucleophilic amino acid residues in proteins and electrophilic products of lipid peroxidation. And if one wishes to characterize those, it is not enough to know the protein and the modification site but also the structure of the lipid peroxidation product (LPP) itself. This challenge became the focus of my Junior Research Group at the Centre for Biotechnology and Biomedicine (BBZ) in Leipzig. Joint by a group of extraordinary Master's and PhD students, over the years we dug deeper and deeper into the fascinating diversity of LPPs, and developed multiple methods for their analysis. Overall, studying the diversity of lipid modifications, both *in vitro* (cell culture) and *in vivo* (animal and human tissues) allowed us to conceptualize the term “epilipidome” as a subset of natural lipidome, formed via enzymatic and non-enzymatic lipid modifications, representing a new level of lipidome complexity required to regulate complex biological functions, similar to epigenetic modifications of DNA and protein PTMs. The concept of epilipidome was readily picked up by the community, and served as a basis for numerous collaborations within COST Action EpiLipidNET, a network of over 450 researchers interested in lipid biology, lipidomics, and lipid modifications!

However, it is difficult to study lipid modifications without knowing what happens to lipids

themselves. So, we had to extend our research even further to lipidomics! Over last year's our group established several high-throughput LC-MS workflows. Last few years we focused especially on setting up a robust and high-throughput method for the in-depth identification and quantification of lipids in animal and human tissues, and blood plasma.

High-throughput LC-MS/MS generates a lot of data! When we started to work with lipids, there were almost no computational tools out there to deal with lipidomics datasets. After a year of manually identifying lipids from tandem mass spectra, Zhixu Ni, a talented scientist in my group, got finally tired and decided to change the focus of his research from wet lab experiments to designing computational solutions for high-throughput processing of lipidomics and epilipidomics datasets. That resulted in the creation of LipidHunter, LPPtiger, and LipidLynxX, a set of lipidomics tools which we call our pride of Big Cats to hunt in the dark forest of lipidomics data.

Having in our hands all the technologies and tools, developed over the last 10 years by many talented and motivated PostDocs, PhD, Master, and Bachelor students in my group, we are now can much better tackle the most complicated questions on the role of lipids in stress responses!

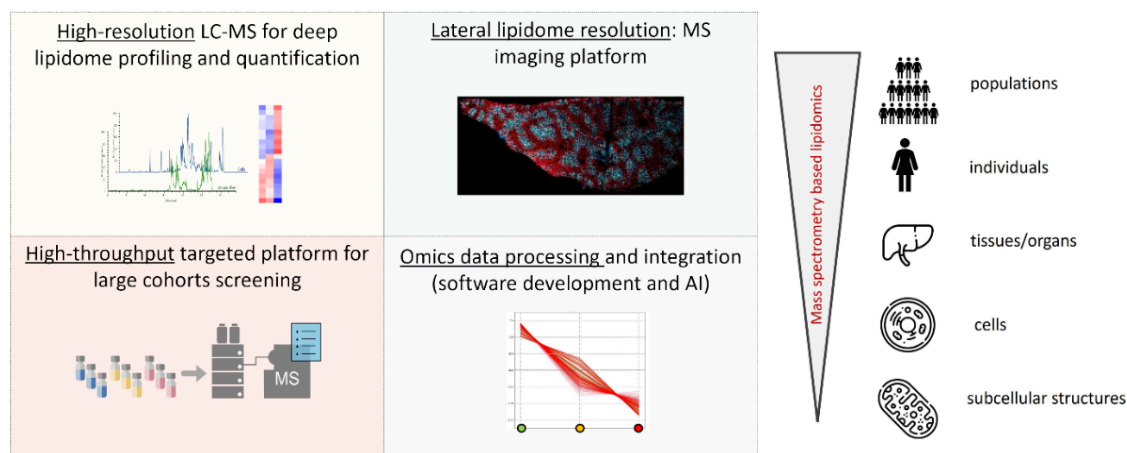


**Research in Fedorova lab with the focus on the role of lipids and lipid quality control in cellular stress responses.**

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

After years of working with MS-based omics, I am still amazed by the fact that we can use MS technology to look into the molecular compositions of any biological system. On a daily basis, within just a few hours from sample extraction to LC-MS/MS analysis, we can "see" hundreds of lipids which form the lipidomes of cells and tissues. Generally, most people (including myself) are very excited about space exploration and technologies related to the research of planetary objects, stars, and galaxies. But if we invert the scale

from macro to micro, we are doing molecular exploration in the lab every single day! We can now characterize the chemical space, and the lipidomes of different tissues and see which lipids make the liver a liver and brain a brain. We challenge cells and see how do they remodel their lipid compositions to adapt to this challenge. We can trace in time and space the localization and abundance of metabolic and signaling molecules, driving the regulatory circuits of Life. That is what makes for me personally the MS-based technologies so exciting, fascinating, and I feel privileged to be able to do it every day in the lab.



**Lipidomics technologies used in Fedorova Lab.**

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

I joined the Technical University of Dresden (TUD) 2 years ago. And one of the main reasons for that was the long-standing history of lipid research and lipidomics in Dresden. Importantly, at **TUD Campus** we have a very strong focus on metabolism, both from basic and biomedical perspectives. This provides a vivid environment and greatly supports the interdisciplinary of the research. As I mentioned above, lipidomics gives us this amazing opportunity to look deep into the molecular making of Life. As exciting as it is, alone it is not enough neither to understand the biology behind nor to explain the pathological complications in biomedical research. And interdisciplinary of biomedical research is exactly the strength and the focus here in Dresden in general and at the [Center of Membrane Biochemistry and Lipid Research](#) (Zentrums für Membranbiochemie und Lipidforschung, ZML).

International, for the last 4 years I was fortunate to be a part of [EpiLipidNET COST Action](#), a Pan-European network in lipidomics and epilipidomics. EpiLipidNET is an international consortium of 450 lipid scientists, clinicians, scientific societies, and enterprises from 47 countries working in the field of lipid research, lipidomics, and lipid modifications. It is supported by the European Cooperation in Science and Technology (COST), which gave

us an amazing opportunity to build and support this network. Over the years, we organized numerous meetings dedicated to lipidomics and epilipidomics analysis, data processing pipelines, clinical translation, and lipid biology. COST program actively supports lab exchange for young researchers via so-called short-term scientific missions, and EpiLipidNET provided funds so support 43 of them so far! I think it is one of our main achievements. Having the opportunity to travel and do research in different laboratories, countries, and environments allows young scientists to see the diversity of scientific approaches, get access to different instrumentation, and build their own professional networks. Recently, our networking activities were highlighted by the COST press release and if you are interested in learning more about what our community achieved via inclusive networking over the last few years, have a short read - <https://www.cost.eu/introducing-lipids-epilipidnet/>. By the way, this year we will host the annual EpiLipidNET Meeting here in Dresden. So, if you are interested in lipids and (epi)lipidomics, you still have time to register. Again, thanks to the COST organization our meetings are free of registration charge. More information about the meeting and the program is available [here](#).

Among the new initiatives I am involved in is a new task group **LipidMet within the Metabolomics Society**, which I have a pleasure to co-chair together with Maria Eugenia Monge (CIBION, Argentina) and Matej Orešič (Örebro University, Sweden and University of Turku, Finland). The rationale behind the LipidMet group is that originally stepping out from metabolomics, lipidomics has grown into a separate field often with its own methods, definitions, and workflows. However, our current understanding of metabolism complexity, its close connectivity, and regulations, calls for integrative solutions bringing back together lipidomics and metabolomics fields. The aim of the LipidMet Task Group within the Metabolomics Society is to bring together the expertise and experiences from both fields and unite them under the common umbrella of metabolism research with shared best practices, harmonization, and quality control protocols.

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

I guess we all wish to contribute to the better future of human society with our research. And the biomedical sector provides a lot of opportunities for such contributions. I certainly hope that our work on human tissue lipidomes will provide an impact on understanding human biology, physiology, and pathologies from the perspective of lipid metabolism. For instance, one of the important aspects, that was overlooked for a long time, is the sex dimorphism of human metabolism. In a project that we are finalizing right now together with our collaborators from Leipzig University (Patricia Prabutzki and Florian Schlotter), we observed amazing differences between male and female manifestations of calcific aortic valve diseases at the molecular level. I think this kind of knowledge is absolutely essential

for the development of personalized therapies, as well as diagnostic and prognostic markers.

There is still so much more to discover in lipidomics signatures! We also look deeply into what we call epilipidome to find new regulatory circuits in physiological and pathological conditions. For instance, with the recently developed methodology, we can now identify oxygenated complex lipids such as phospholipids, cholesteryl esters, and triacylglycerides in circulating lipoproteins, which probably serve as a carrier of bioactive oxylipins. The availability of these new analytical pipelines which my group developed over the last few years, will allow us to “trace” what kind of oxylipins are carried, from where, and to which destinations. Considering the high significance of these bioactive lipids in a wide range of inflammatory conditions, it is important to know which signals and at which pathophysiological conditions for instance liver sends into the circulations and by which tissues these signals are received.

### **As you see it, what are lipidomics' greatest strengths?**

The strength of modern lipidomics is that over the last decade, the field has become mature enough to provide solid, robust, and reproducible data. It is very important if we want lipidomics to be “taken seriously” both in basic and translational research. With great community-driven efforts by Lipidomics Standard Initiative and Quality Assurance and Quality Control Consortium, many measures to ensure data quality are provided and available to everyone. We can now generate “big” lipidomics data in a way that they are comparable with the studies made by others. This means that one lab does not need to do it all, but can use publicly available datasets produced by other researchers. In this respect, I would like to underline the significance of data sharing and providing your raw and metadata upon publication via open-access repositories.

### **What do you see as the greatest barriers for lipidomics?**

To me, the greatest barrier for lipidomics is data integration toward providing biological meaningful answers. With the great hardware technologies and analytical pipelines in our hands, we generate large and very detailed sets of lipidomics data. But the explanation, of what it means in the biology sense is still not easy to find. I wish we could move the field further towards more interdisciplinary research where it will be common for lipidomics, metabolomics, and proteomics experts to work directly together with biochemists, cell biologists, clinicians, and bioinformaticians together to solve a particular riddle in the biomedical field.

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

I think both metabolomics and lipidomics have taken off already. The significance and inputs these fields provide are illustrated by numerous examples related to understanding the pathological trajectories in metabolic, degenerative, and malignant diseases. As I mentioned above, thanks to the community-driven efforts we are much better in terms of standardization and harmonization of our analytical workflows. It is also important to make this a part of the educational curriculums in the fields of analytical chemistry, lipidomics, and metabolomics. One of the very attractive directions for lipidomics is its clinical translation. In this case especially, the standardization and quality control of analytical workflows are a must.

On a very particular note, I wish we could have access to a larger number of chemically defined isotopically labeled standards for various lipids and their modified forms. It still remains one of the major bottlenecks in setting up quantitative lipidomics workflow. It is clear that we cannot have a standard for each lipid in complex lipidomes. So maybe we should invest more in developing computational solutions based on machine learning models to provide a reliable response factor we can use for quantification purposes.

Finally, I would like to underline the importance of the open science approach. As a community, sharing the data, methods, and tools, will allow us to use our time and resources much more efficiently without reinventing the same workflows or re-measuring the same type of samples over and over again. The community can benefit greatly by sharing and having access to global knowledge and expertise!



**Members of Fedorova lab and visiting researchers**  
**(Image Copyright: Michele Wölk)**

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# Metabolomics and Multi-omics Data Analysis

This service provides advice and guidance on how to use **MetaboAnalyst** for targeted or untargeted metabolomics data analysis, as well as how to link metabolomics with other omics data such as transcriptome and microbiome



## Recent Publications

### Reviews:

- [Breaking bugs: gut microbes metabolize dietary components and modulate vascular health](#)
- [Metabolomics-centered mining of plant metabolic diversity and function: Past decade and future perspectives](#) (Open access)

- [Metabolomics and lipidomics strategies in modern drug discovery and development](#)
- [The expanding diagnostic toolbox for rare genetic diseases](#)

## **Articles:**

- [3D superstructure based metabolite profiling for glaucoma diagnosis](#) (Open access)
- [A conserved interdomain microbial network underpins cadaver decomposition despite environmental variables](#) (Open access)
- [A machine learning approach for understanding the metabolomics response of children with autism spectrum disorder to medical cannabis treatment](#) (Open access)
- [A spectroscopic test suggests that fragment ion structure annotations in MS/MS libraries are frequently incorrect](#) (Open access)
- [Differential peripheral immune signatures elicited by vegan versus ketogenic diets in humans](#) (Open access)
- [Environmentally relevant concentrations of chemically complex shale gas wastewater led to reduced fitness of water fleas \(\*Daphnia carinata\*\): Multiple lines of evidence approach](#) (Open access)
- [Evaluation of normalization strategies for GC-based metabolomics](#)
- [HDPairFinder: A data processing platform for hydrogen/deuterium isotopic labeling-based nontargeted analysis of trace-level amino-containing chemicals in environmental water](#)
- [Human microbiota from drug-naïve patients with obsessive-compulsive disorder drives behavioral symptoms and neuroinflammation via succinic acid in mice](#)
- [Integrated spatial transcriptomics and lipidomics of precursor lesions of pancreatic cancer identifies enrichment of long chain sulfatide biosynthesis as an early metabolic alteration](#)
- [Lipidomics Profiling of Metformin-Induced Changes in Obesity and Type 2 Diabetes Mellitus: Insights and Biomarker Potential](#) (Open access)
- [Multi-Omics Reveals the Genetic and Metabolomic Architecture of Chirality Directed Stem Cell Lineage Diversification](#) (Open access)
- [Per- and Polyfluoroalkyl Substances Concentrations are Associated with an Unfavorable Cardio-Metabolic Risk Profile: Findings from Two Population-Based Cohort Studies](#) (Open access)
- [SAND: Automated Time-Domain Modeling of NMR Spectra Applied to Metabolite Quantification](#)
- [Tryptophan sulfonate: A new chemical marker for accurate and efficient inspection of sulfur-treated food products](#)
- [Untargeted metabolomics analysis of non-volatile metabolites and dynamic changes of antioxidant capacity in Douchi with edible mushroom by-products](#)

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## **MANA SODAMeet**

**April 9, 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 # 03: Mass Spectrometry Imaging 101: Sample Preparation**

**April 11, 2024**

**Venue: Online**

Bits & Bites 2024 is a flexible learning experience tailored for busy researchers seeking condensed yet impactful sessions. Now in its fourth year, this series continues to bridge the gap for those unable to commit to 1- or 2-week intensive courses.

10-part short course series will feature in-depth topics in untargeted metabolomics such as mass spectrometry applications, mass spectrometry imaging, statistics with both MetaboAnalyst and R, GNPS, MS-DIAL, and so many others. Each short course can be taken individually or you can select multiple Bites. Participants 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 a highly interactive manner, with the use of freely available software and databases. The tuition is \$175 USD per Bite, except for #10. The tuition for #10 is \$350 USD as it will take approximately 8 hours.

This 3rd course is led by Dr. Elizabeth Neumann from UC Davis, and offers an introductory look into the fundamentals of mass spectrometry imaging (MSI), with a focus on sample preparation techniques like tissue freezing, sectioning, and matrix application. Tailored for beginners with no required software or prerequisites, this short course aims to equip participants with essential skills in MSI instrumentation, data analysis, and visualization, providing a solid starting point for researchers and students embarking on MSI projects.

[Check for more details](#)

## **X-omics festival 2024**

**April 15, 2024**

**Venue: Nijmegen, Netherlands**

The sixth edition of the X-omics festival “The future of multi-omics research is now!” will include:

- A keynote lecture
- Lectures from X-omics investigators on the X-omics facilities, innovative technologies, multi-omics data integration and multi-omics impact
- User pitches about innovative omics technologies
- A pitch your project session with the expert panel
- Scientific posters and poster pitches
- Networking opportunities

Registration for the X-omics festival 2024 is free of charge but required to attend the event.

[Check for more details](#)

## **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.

[Check for more details](#)

## 5th Annual Canadian Metabolomics Conference (CanMetCon) 2024

**April 25 – 26, 2024**

**Venue: Vancouver, Canada**

The 5th Annual Canadian Metabolomics Conference (CanMetCon) 2024 will be held in April 25-26, 2024 at the University of British Columbia, Vancouver, BC, Canada. This year, the conference presents an exciting two-day agenda: Day 1 is dedicated to "Metabolomics Technology and Integration", offering deep dives into the latest advancements and methodologies, while Day 2 focuses on "Multiomics and Applications". Registration for the conference is open, inviting researchers, students, and professionals to join this vibrant gathering of the metabolomics community!

Important dates:

- Early Bird Registration deadline: **February 29, 2024**
- [Abstract Submission](#) Deadline: **March 15, 2024** to be considered for Oral Presentation  
**March 22, 2024** for Posters
- Registration Deadline: **March 22, 2024**

Early bird registration fees are CAD 150 for students and CAD 250 plus applicable taxes and fees. Your registration fee includes a welcome reception on April 25, breakfast and lunch on April 25–26, and light refreshments during morning and afternoon coffee breaks.

Check out our updated conference program [here](#).

[Register now](#)

## 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. Save the upcoming dates:

- Abstract submission is open
- Oral Abstract deadline: March 7, 2024
- 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, glycomics etc.
- MS data processing and Informatics

Registration is [open](#) now and will close on **June 12, 2024**.

For more information, please visit [msbm.org](https://msbm.org) or send an email to [msbm.dubrovnik@gmail.com](mailto:msbm.dubrovnik@gmail.com)

[Learn more here](#)

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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>

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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
Growth and Outreach Coordinator	The Metabolomics Innovation Centre, University of Alberta	Edmonton, AB, Canada	<a href="#">The Metabolomics Innovation Centre (TMIC)</a>
Postdoctoral Fellow – Microsampling devices for lipidomics	Concordia University	Montreal, QC, Canada	<a href="#">The Metabolomics Innovation Centre (TMIC)</a>
Postdoctoral Research Associate in Metastasis Metabolism	Nuffield Department of Surgical Sciences , University of Oxford	Oxford, UK	<a href="#">Metabolomics Society</a>
Experimental Officer in Metabolomics	School of Biosciences, University of Birmingham	Edgbaston, Birmingham, UK	<a href="#">Metabolomics Society</a>
Canada Research Chair (CRC) Tier 2 in Metabolomics	Schulich School of Medicine and Dentistry, Western University	London, ON, Canada	<a href="#">Western University</a>
Chemical Biologist/Ecologist	The Monell Chemical Senses Center	Philadelphia, PA, USA	<a href="#">The Monell Chemical Senses Center</a>
ORISE Postdoctoral Fellowship in Pharmacology/Toxicology	National Center for Toxicological Research U.S. Food and Drug Administration	Jefferson, AR, USA	<a href="#">Metabolomics Society</a>
ORISE Postdoctoral Fellowship in Neuroscience/	National Center for Toxicological Research	Jefferson, AR, USA	<a href="#">Metabolomics Society</a>

Neurotoxicology	U.S. Food and Drug Administration		
Post-Doctoral Fellow	Department of Medical Microbiology & Immunology, University of Alberta	Edmonton, AB, Canada	<a href="#">University of Alberta Careers</a>
Operations Assistant	NovaMT and TMIC Li Node at the University of Alberta	Edmonton, Alberta, Canada	Dr. Liang Li (please contact <a href="mailto:liang.li@ualberta.ca">liang.li@ualberta.ca</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>

## 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](mailto:metabolomics.innovation@gmail.com)

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