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# MetaboNews

### This month in metabolomics

June, 2024 Vol 14, Issue 6

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





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Matej Orešič

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# **Metabolomics Society News**



METABOLOMICS SOCIETY

FARIY- CAREER MEMBERS NETWORK

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

**General Enquiries** 

info@metabolomicssociety.org

## **Members' Corner**

#### **Board of Directors**

Dear Society Members,

By the time this is out in 'print' we shall either be in Osaka enjoying metabolomics science and Japanese hospitality or reflecting on an excellent and memorable event.

In my last message to you, and in our Town Hall meeting on Monday evening (17 June 7-8 pm; Osaka time), we discussed the positions available to serve on the Board of Directors of the Metabolomics Society.

A reminder that the Board comprises 13 elected board members and these include three Officer positions – President, Treasurer and Secretary. We are also joined by the chair of the Early Members Network (Silvia) and up to 3 immediate past Officers (non-voting members). This year there are 7 vacancies and thus 7 Directors to be elected. Fabien and I as Secretary and President will become past Officers, and so will be retained for 2 years to help during the transition to the new Board and Officers. This also means that there will be a need to vote for a new President and new Secretary.

As stated on our website our Society is an independent, non-profit organization, governed by a Board of Directors. This BoD is composed of dedicated members of the metabolomics community who are ultimately responsive to its members. Our mantra is to promote and to enhance metabolomics globally. The Director's duties are many and varied and include helping with our conference, leading Society Committees as well as providing input into our Scientific and other Society Task Groups. The Directors positions are voluntary and involve monthly online meetings to run the Society. The work is fun and varied. Personally I have found it an honour to serve the society. The commitment to helping, being enthusiastic and active is an important aspect for these BoD positions. The Society has grown and has more than 1000 members in over 40 countries, so it is important that the board serve our membership well.

If you want to get involved and feel you have the time to do this then do. It is a great experience!

The timelines of our elections are highlighted below:

For the seven new Director positions –

- Call for Nominations are from 25 June to 18 July
- Statements and Bios are due by 22 July
- Election Poll Open from 29 July through to 20 August

Once the new Board has been formed then the President and Secretary positions needed to be decided. The timeline is as follows –

- Call for Officer Nominations from 23 August to 4 September
- Officer Bios and Statement are due by 9 September
- Voting for the two Officers from 12-25 September

The new term for the new Board will begin 1 October 2024.

Please do consider getting involved and please reach out to any of the current directors if you would like to know more about this opportunity to serve the Metabolomics Society. <a href="https://metabolomicssociety.org/board-committees/board-of-directors/">https://metabolomicssociety.org/board-committees/board-of-directors/</a>

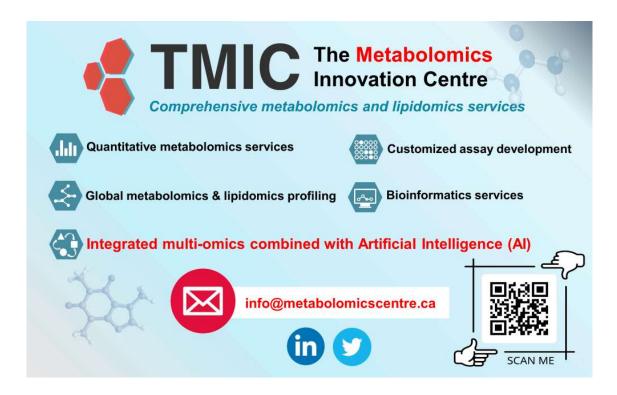
All members of the society will receive details of the Call for Nominations process and be reminded of the above timings for the Voting Poll periods.

Remember Your Society needs You!

All the very best.

Roy Goodacre, University of Liverpool, UK

**President, Metabolomics Society** 



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

These assays cover a wide range of metabolites and analytical techniques, including targeted and untargeted approaches by using the most comprehensive set of technologies: NMR, CE-MS, GCxGC MS, GC-MS, LC-MS, UPLC, HPLC, and mass spectrometry imaging. Also, offering customizable

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

#### **Early-career Members Network (EMN)**

#### **EMN Accepting Applications!**

This summer, EMN will be receiving applications from early career metabolomics researchers. The applicants need to be either currently enrolled in a graduate program, or be less than 5 years from obtaining their PhD degree to be considered. In addition, applicants need to be members of the metabolomics society at the time of the application. This year we have 5 open positions. The 2-year mandate of each EMN representative will run from October 2024 to October 2026. The applications will open in early August. Keep an eye on our updates on <a href="twitter">twitter</a> (@EMN\_MetSoc) or/and <a href="tinkedin">linkedin</a>!

#### **EMN Webinars**

The EMN would like to once again thanks Prof. Nicholas JW Rattray for his insightful and brilliant talks on Biomarkers discovery in metabolomics in our May webinar. The webinars will be interrupted during the summer break and will resume in September at a date and time to be determined. We will keep you posted! In the meantime, we wish you a nice summer break!

#### EMN at Metabolomics 2024 in Osaka:

#### **EMN Events**

The EMN would like to thank the Career Night speakers: Natasa Giallourou, Michael Witting, Farhana Pinu, Alice Limonciel, Jules Griffin, Masanori Arita, Audrey Le Gouellec, Tomáš Pluskal, Nicholas Rattray, Dajana Vuckovic, Eiichiro Fukusaki, Marissa Jones, Postdoc Yasmine Hamany, Postdoc Helena Mannochio Russo, Timothy Ebbels, Bart Ghesquière, David Beale, Kyo Bin Kang, Pieter Dorrestein, Fidele Tugizimana, Sandi Azab, Stefania Noerman and the panelists of the EMN Career Develoment Workshop: Natasa Giallourou, Emma Schymanski, Tomáš Pluskal, Ian Castro-Gamboa, Pieter Dorrestein that made our events a great succes. We also would like to thank all ECRs for their participation in our events during Metabolomics2024: Career Night, the EMN Workshop and also the EMN Reception. In addition, we would like to thank you for stopping by our booth to find out about the activities we offer throughout the year. We hope you enjoyed it as much as we did!

#### **EMN MetaboART**

EMN MetaboART winners have been announced at the Metabolomics conference in

Osaka, during the EMN reception. Once again, we want to congratulate Domenica Berrardi (1st place), Laimdota Zizmare (2nd place) and Diana Vinchira (3rd place). We also thank all the participants for sending in their work.

#### **EMN Travel Bursary**

We are happy to announce the 4 awardees of the EMN Travel bursary for the Metabolomics Society conference that took place in Osaka 2024. Two of the graduate travel awards were given to Graduate students **Novia Minae** (*Centre for Computational and Systems Medicine, Australian National Phenome Centre, Murdoch University*) and **Marina Botana** (*School of Biological Sciences, Victoria University of Wellington, New Zealand & Institutet för Miljömedicin, Karolinska Institutet, Sweden*). Two of the postdoc awards were given to **Alex Castro** (*Brazilian Center for Research in Energy and Materials* (*CNPEM*), *Brazilian Biosciences National Laboratory* (*LNBio*), *Campinas, SP, Brazil*) and **Yasmine Hamany Djande** (*University of Johannesburg in South Africa, faculty of Science, department of Biochemistry*).

The award was presented to the awardees at the closing ceremony of the conference. We wish our awardees a lot of success with their future research!



### **International Affiliates' Corner**

## Australia & New Zealand Metabolomics Society (ANZMetSoc)

Visit: <a href="https://anzmetabolomics.org/what-we-do">https://anzmetabolomics.org/what-we-do</a>

The Metabolomics Australia facility at the University of Melbourne, funded by NCRIS and

institutional support, is on the lookout for a Technical Assistant!

Join one of the largest and most advanced metabolomics facilities in Australia, providing cutting-edge mass spectrometry-based services to academia, industry, and government.

If you're passionate about advancing metabolomics research and eager to work with toptier instrumentation, this is the role for you!

Apply now and be part of a dynamic team at the forefront of scientific discovery. https://lnkd.in/gBP4SqYD

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

Visit: <a href="http://www.rfmf.fr/">http://www.rfmf.fr/</a>



# The Breton sun was shining bright on the 16th RFMF Scientific Days

Dear colleagues and participants of the 16th Scientific Days of the French-speaking Metabolomics and Fluxomics Network,



It was with great pleasure that **289 metabolomicists gathered in Saint Malo** to celebrate metabolomics and the development of our community. The international speakers, oral presentations, flash communications and 135 posters were of exceptional quality, testifying to the excellence of our work.

Among the highlights, we also elected **Estelle PUJOS GUILLOT** as a 2023 honorary **member**, and the Rolin Portais prize was awarded to **Juliette COOKE**.

We would like to thank the local committee, in particular Alain BOUCHEREAU, Pauline

**LE BOULCH** and **Anne LEVREL**, as well as our local organization group, particularly **Marine LETERTRE**, and all the colleagues involved, for their dedication and attention, which made this event so special.

We would also like to **thank all our sponsors**, without whom this event could not have taken place.

Next year will mark the **20th anniversary of the RFMF**, and we warmly invite you to **join us in Paris from 10 to 13 June 2025** to celebrate. We look forward to seeing you next year! Audrey **LE GOUELLEC**, your delighted President and the entire Board of Directors (having fun on the picture below;))





### Metabolomics Association of North America (MANA)

Visit: <a href="https://metabolomicsna.org">https://metabolomicsna.org</a>

Email <u>mana@metabolomicsna.org</u>

LinkedIn @MANA (Metabolomics Association of North America)

X <u>@MetabolomicsANA</u>

Save the date for our 6th Annual MANA Conference! This year, the meeting will be in Tampa, Florida, USA, October 21-24, 2024. Abstract submissions are now open (*Oral deadline July 19 and Poster Aug. 16*)! Please visit our website at <a href="https://pwd.aa.ufl.edu/mana/">https://pwd.aa.ufl.edu/mana/</a> for more details. Awards opportunities will be announced soon.

Be sure to also check out our news and events pages for more information on activities from MANA interest groups and committees. Recent and upcoming MANA members-led activities include:

- Interactive SODA (SOftware and DAta Exchange) Meetups (see here for recordings)
- NIH Workshop in Metabolomics Epidemiology took place on May 15, 2024, featuring our MANA President and ECM Vice Chair as speakers.
- The NMR Interest group published a perspective piece on using and reusing NMRbased metabolomics data: see <u>Gouveia et al. Metabolomics 2024</u>.

Remember to also visit our job board for open positions in metabolomics.

## **Scottish Metabolomics Society**

Visit: http://www.scottishmetabolomics.net/

The Scottish Metabolomics Network will host its annual symposium on the 22<sup>nd</sup> and 23<sup>rd</sup> of October 2024 within the Institute of Aquaculture at the University of Stirling. There will be a range of talks and posters on all aspects of metabolomics and local and international metabolomics researchers are encouraged to visit Stirling and experience its rich medieval history and stunning scenery. On the Monday before the event (21<sup>st</sup>) there will also be a hands on chemometrics training workshop aim at developing stats skills for ECRs.

Other items from the SMN| SUERC – Centre for the Isotope Sciences at The University of Glasgow has recently installed the new ThermoFisher Orbitrap Exploris isotope Solutions 480 mass spectrometer (MS) which brings unrivalled sensitivity and precision

to high resolution isotope ratio MS. Supported by a recent UKRI BBSRC Pioneer award to Professor Douglas Morrison at SUERC, this platform will open up new avenues in ultra-low tracer and natural isotopologue studies in biological systems.

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# Our passion is helping scientists follow theirs.

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# Metabolnterview

# Matej Orešič



Professor of Medicine (Systems Medicine). School of Medical Sciences, Örebro University, Örebro, Sweden

Professor of Biochemistry (Metabolomics). Turku Bioscience Centre and Department of Life Technologies, University of Turku, Turku, Finland

Coordinator, INITIALISE EU project

Co-Coordinator, EDC-MASLD EU project

# **Biography**

Matej Orešič holds a PhD in biophysics from Cornell University (1999; Ithaca, NY, USA). He is professor of medicine (systems medicine) at Örebro University (Sweden) and professor of biochemistry (metabolomics) at the University of Turku (Finland). Prof. Orešič's main research areas include exposomics and metabolomics applications in biomedical research and systems medicine. He is particularly interested in the

identification of environmental exposures (exposome) and disease processes associated with different metabolic phenotypes and the underlying mechanisms linking these processes with the development of specific disorders or their co-morbidities. Prof. Orešič also initiated the popular MZmine open-source project, which led to the development and release of popular software for metabolomics data processing. As of 2016, he was made a Lifetime Honorary Fellow of the Metabolomics Society. Professor Orešič currently serves as member of the Board of Directors of the Metabolomics Society and is one of the founders of the Nordic Metabolomics Society, previously serving as its chair of the board. Within the Metabolomics Society, he chairs the International Affiliates Task Group and is co-founder and secretary of the Lipidomics Task Group (LipidMet).

In 2019, he co-chaired the 1st Gordon Research Conference on 'Metabolomics and Human Health' (Ventura, CA, USA). Previously, he also chaired the Keystone Symposium on Systems Biology of Lipid Metabolism (2015; Breckenridge, CO, USA). Professor Orešič currently coordinates Horizon Europe project "Inflammation in human early life: targeting impacts on life-course health – INITIALISE". He is also Vice-Coordinator of the new Horizon Europe project "Investigation of endocrine-disrupting chemicals as contributors to progression of metabolic dysfunction-associated steatotic liver disease – EDC-MASLD".

#### How did you get involved in metabolomics?

I started my career as a theoretical physicist at University of Ljubljana in Slovenia, then completed my PhD studies in the field of biophysics at Cornell University. In 2001 I joined Beyond Genomics, a start-up company in Boston area which was one of the first companies adopting a systems biology approach in biomedical R&D. While being primarily involved in leading the developments of the biocomputational pipeline in the company, I soon realized how centrally important the data acquired from metabolomics platforms was. After moving to Finland in 2003, I established my own research team in the area of systems biology. The technology platform that we chose to establish ourselves was mass spectrometry (MS) - based metabolomics. At the time there were no satisfactory solutions for metabolomics data processing beyond 'black box' solutions, thus as part of the metabolomics platform development, we also released the open source data processing software MZmine. First version of MZmine was made in 2004, therefore, this year we are celebrating 20 years of MZmine. Over the years, MZmine became a truly community-driven effort which importantly contributed to the growth of the computational MS field.

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

In my 'early days' of metabolomics, methodological developments, particularly on the computational side, comprised a significant fraction of my research. As of late, there has been more emphasis on the applications of metabolomics and on ways to integrate multiomics data in biological context. There is of course a need to continuously improve analytical methods and data processing workflows. In our research, under the guidance of Professor Tuulia Hyötyläinen, we deploy targeted (quantitative) as well as semi- or untargeted approaches, including 'hybrid' targeted and untargeted, and the methods have been recently expanded to cover broad range of environmental chemicals. With the new infrastructure that we have available, including for MS imaging in Turku, there are new opportunities for the methodological developments and applications.

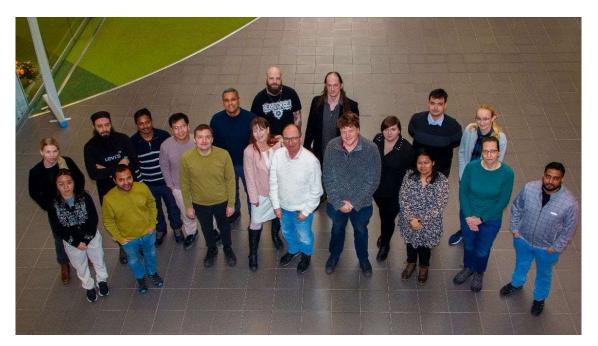
Over the past years, one productive area of our research has been the studies of how chemical exposures (exposome) impact metabolome and gut microbiome, and how these internal exposures, in turn, impact various health outcomes. Our most recent research suggests that chemical exposures have marked impact on metabolism even *in utero*, with potential long-term consequences (Hyötyläinen T, et al. <u>In utero exposures to perfluoroalkyl substances and the human fetal liver metabolome in Scotland: a cross-sectional study</u>. Lancet Planet Health. 2024 Jan;8(1):e5-e17).

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

I am involved in coordination of two European collaborative projects. Horizon Europe project "Inflammation in human early life: targeting impacts on life-course health — INITIALISE", which started in 2023, aims to elucidate how the immune system is imprinted due to various external and internal exposures in early life, and how, in turn, such imprinting impacts lifecourse health. Metabolomics, which includes analyses of chemical exposome, is one of the key analytical platforms applied, alongside, proteomics, shotgun metagenomics (gut microbiome), genetics/genomics, and single-cell omics. Such a multi-omics approach is applied in several prospective clinical cohorts. The project already led to some important findings that were published this year (Ahrens AP, et al. Infant microbes and metabolites point to childhood neurodevelopmental disorders. Cell. 2024 Apr 11;187(8):1853-1873.e15, and Hyötyläinen T, et al. In utero exposures to perfluoroalkyl substances and the human fetal liver metabolome in Scotland: a cross-sectional study. Lancet Planet Health. 2024 Jan;8(1):e5-e17).

The Horizon Europe project "Investigation of endocrine-disrupting chemicals as contributors to progression of metabolic dysfunction-associated steatotic liver disease – <u>EDC-MASLD</u>", which started this year, builds on three previous European projects (FLIP, EpoS, and most recently IMI2 project LITMUS) that assembled a cohort of over 9,000 histologically characterized patients with metabolic dysfunction-associated steatotic liver

disease (MASLD), of which over 6,000 are being longitudinally followed-up. While there is some evidence suggesting that endocrine-disrupting chemicals (EDCs) contribute to steatosis, little is known about the contribution of EDCs to transitions towards the more advanced stages of MASLD. The overall aim of EDC-MASLD is to elucidate the role of EDCs in the initiation and progression of MASLD.



The Orešič research group from Örebro University and University of Turku.

#### What is happening in your country in terms of metabolomics?

I currently lead research teams both in Finland and Sweden (which work closely together), and was previously also working as a PI in Denmark for few years. There are certainly some differences between the Nordic countries when it comes to national funding opportunities and infrastructure investments, but in general metabolomics has been getting recognition by the funders and institutions. Within the Nordic region comprising five countries, we have the Nordic Metabolomics Society, which has its annual conference this year in Turku, Finland in late August (<a href="https://nmetc2024.fi/">https://nmetc2024.fi/</a>). Our meetings typically attract 150-200 researchers from the Nordic region and beyond, although based on the number of submitted abstracts this year, the meeting in Turku may exceed these numbers. There is clearly growing interest in metabolomics in the region, in line with the global growth of the field.

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

Recently reported findings that the chemical diversity of metabolome (*e.g.*, bile acids, N-acyl amides) is considerably larger than previously thought requires a rethink of biochemistry and possibly physiology. There is also a need to develop analytical protocols with broad coverage of these lipid sub-classes. We approached this new

challenge by pursuing developments of both new targeted and untargeted protocols for analyses of these metabolites, similarly as we did for the analyses of chemical exposome. At the Metabolomics 2024 conference in Osaka, I presented first results utilizing the extended targeted platform for analysis of bile acids, including new conjugates, in the context of early life and future progression to type 1 diabetes. In general, our work such as currently pursued in INITIALISE and EDC-MASLD projects as well as in other related projects may help elucidate the environmental factors and early pathophysiological mechanisms contributing to the future diseases. Such knowledge may inform about the disease prevention strategies.

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

While metabolome is increasingly being recognized as an important mediator between the exposome and life course health, the greatest strength of metabolomics seems to be that there are still so many persisting unknowns. Our biochemistry is largely still being based on key research done half a century or more ago, despite currently witnessing great advances in instruments as well as in analytical and computational methods that are enabling study of metabolome with ever greater accuracy, sensitivity, and coverage. There is still a lot to be discovered.

#### What do you see as the greatest barriers for metabolomics?

Metabolomics community, which in broad sense includes other communities such as lipidomics, is historically highly diverse. This is a particular strength of the field that will further contribute to its growth. Nevertheless, if there was not enough communication between the historically separate subfields of metabolomics, this could also present potential barriers, *e.g.*, in the development of common reporting standards. I feel that the field is advancing so fast now that these potential barriers, if existing, will disappear.

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

It has already taken off.

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

With the new methodological developments and opening of new application areas, metabolomics is thriving. This is reflected also by having more funding opportunities where metabolomics can be included, even if not as a primary analytical platform. I am involved in leading a metabolomics service facility (Turku Metabolomics Centre), and

there has clearly been an increased interest in applying metabolomics in various funding applications.

#### What role can metabolomics standards play?

Metabolomics Standards Initiative (MSI) has been very important for the advance of the metabolomics field and the core principles set by MSI still apply. Despite aging well, given the growth of the field over the years, an update of MSI is warranted. As part of this, it would be important to engage a broad metabolomics community, including, e.g., lipidomics and MS imaging. In order to facilitate such much needed communication, we recently set up LipidMet Task Group of the Metabolomics Society. Regarding the standards in general, for best compliance, pragmatism is the key. There is a difference between setting up a diagnostic panel for regulatory approval vs. a discovery study involving broad suspect screening of environmental chemicals as well as metabolites. Given the rapid growth of the field and the technologies, standards should not explicitly or implicitly make preferences for specific analytical approaches, neither be too complex to adopt in real-life settings. One area where significant improvements could be made is agreement about the use of common reference samples for QC (e.g., NIST SRM 1950 for analyses of plasma samples) and use of a minimal set of internal standards for analyses of specific groups of metabolites. This would improve comparability of results.

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# Micro-credential in Metabolomics @ UBC

Develop the skills to discover, identify, and quantify metabolites in any biological sample over the span of this 39-hour micro-credential.

Enrolment opens April 15th, closing July 15th, with the course running August 6th - 16th, 2024.

For more information about the course, its structure and delivery, and learning outcomes, please visit: cpe.ok.ubc.ca/courses/metabolomics





### The Metabolomist Podcast



## New episode

Aging fluidity & omics signatures

I cannot think of a more important topic [than aging] because biomedical research is organized around diseases like cancer, Alzheimer's disease, cardiovascular disease... where the incidence increases exponentially with age. Age is by far the main risk factor. So if we understand aging and try to influence it, it could delay the onset of all of these diseases at once. The impact would be huge. Not comparable to anything that we've known in medicine.

-Vadim Gladyshev

LISTEN NOW



### **Recent Publications**

# **Reviews:**

- Aging-Related Sarcopenia: Metabolic Characteristics and Therapeutic Strategies
- Frontiers in mass spectrometry-based spatial metabolomics: Current applications and challenges in the context of biomedical research (Open access)
- Heavy arch: from inflammatory bowel diseases to metabolic disorders
- Metabolic remodelling in atrial fibrillation: manifestations, mechanisms and clinical implications

## **Articles:**

- <u>Benchtop volatilomics supercharged: How machine learning based design of experiment helps optimizing untargeted GC-IMS gas phase metabolomics</u>
- Colorectal cancer microbiome programs DNA methylation of host cells by affecting methyl donor metabolism (Open access)
- <u>Difference in muscle metabolism caused by metabolism disorder of rainbow trout liver</u> <u>exposed to ammonia stress</u>
- Ectomycorrhizal fungi alter soil food webs and the functional potential of bacterial communities (Open access)
- <u>Integrated proteomic, transcriptomic, and metabolomic profiling reveals that the</u> <u>gibberellin-abscisic acid hub runs flower development in the Chinese orchid Cymbidium sinense</u> (Open access)
- <u>Integrative metabolomics-genomics analysis identifies key networks in a stem cell-based model of schizophrenia</u> (Open access)
- <u>Lipid-based insulin-resistance markers predict cardiovascular events in metabolic dysfunction associated steatotic liver disease</u> (Open access)
- Metabolomic analysis of rumen-protected branched-chain amino acids in primiparous dairy cows
- Metabolomics profiling reveals distinct, sex-specific signatures in serum and brain metabolomes in mouse models of Alzheimer's disease (Open access)
- NMR and LC-MS-based metabolomics to investigate the efficacy of a commercial bio stimulant for the treatment of wheat (Triticum aestivum) (Open access)
- <u>Smoking cessation only partially reverses cardiac metabolic and structural remodeling in mice</u> (Open access)
- Suspect screening analysis by tandem mass spectra from metabolomics to exposomics
- <u>Metabolites are overlooked in environmental risk assessments and monitoring of</u> pharmaceuticals: The case study of pantoprazole
- <u>To analyze the relationship between gut microbiota, metabolites and migraine: a two-sample Mendelian randomization study</u>

 WebGestalt 2024: faster gene set analysis and new support for metabolomics and multiomics (Open access)

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# **Metabolomics Events**



#### **MANA SODAMeet**

July 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

# 16th Mass Spectrometry School in Biotechnology and Medicine

July 7 - 13, 2024

Venue: Dubrovnik, Croatia

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

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

For more information, please visit msbm.org or send an email to msbm.dubrovnik@gmail.com



International Theoretical and Practical Course: "Making Metabolomics Matter: Targeted Approaches for Translational and Precision Medicine"

July 22 - 26, 2024

Venue: Facultad de Química, Universidad Nacional Autónoma de México (UNAM). Cto.

Escola S/N, C.U., Coyoacán, 04510 Ciudad de México, CDMX (In-person)

The course will include education and hands-on training in metabolomics, from experimental design and sample preparation, to running the instrumentation, analyzing the data, and interpreting the results. The principal objective is to emphasize how metabolomics (the most recent omics discipline) could help in the understanding of metabolic perturbations which are the origin of several diseases. Due to its heterogeneity and a complex genetic background, in some populations, such as Mexican and Latin American populations, personalized medicine could be a feasible alternative for getting more adequate diagnosis and treatments. By applying innovative biotechnology products, the students will learn how targeted metabolomics uses the FAIR principles for scientific data, which is Findability, Accessibility, Interoperability and Reusability (FAIR), with pivotal importance for large studies trying to find biomarkers for the diagnosis or prognosis of multiple diseases.

Course Coordinators: Dr. Yamilé López Hernández and Dr. Osbaldo Resendis Antonio.

Learn more here

#### Micro-credential in Metabolomics

August 6 - 16, 2024

**Venue: University of British Columbia (Online)** 

This learning opportunity is designed for professionals who have typically earned an undergraduate degree or college diploma in a science or engineering discipline and are engaged in continuing professional development.

Participants successfully completing the course will have knowledge, skills, and competencies in:

- Metabolomics tools, instruments, software and methodologies
- Experimental design, standardization, and eliminating bias in metabolomics
- Data generation, curation, integrity and quality assessment
- Compound identification and discovery
- Univariate and multivariate statistical approaches
- Biochemical pathway mapping, metabolite clusters, and metabolomics data interpretation
- · Scientific literature reporting metabolomics findings
- Applications of metabolomics

Enrollment Period: April 15 - July 29, 2024

For more information please visit: <a href="mailto:cpe.ok.ubc.ca/courses/metabolomics">cpe.ok.ubc.ca/courses/metabolomics</a>

Learn more here

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

**September 12, 2024** 

Venue: Online

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

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

Check for more details



# Bits & Bites # 07: Using MetaboAnalyst for Metabolomics Statistics and Data Visualizations October 3, 2024

**Venue: Online** 

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

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

**Check for more details** 

# **Metabolomics in Toxicology course**

October 7 – 9, 2024

Venue: School of Biosciences - University of Birmingham

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

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

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

Learn more here

# Untargeted Metabolomics LC/MS Data Processing course

October 14-16, 2024

Venue: School of Biosciences - University of Birmingham

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

Delegates will be provided with real LC-MS datasets for hands-on analysis, and throughout several sessions will be guided through various tools for metabolomic data processing and

statistical analysis, including XCMS, univariate statistics, multivariate analysis, and annotation processing.

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

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.

# **Metabolomics Jobs**

# **Metabolomics Jobs**

If you have a job to post, please email the MetaboNews team at <a href="metabolomics.innovation@gmail.com">metabolomics.innovation@gmail.com</a>

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
Junior Group Leader, Plant Metabolomics	MetaCom, Institute for Plant Biochemistry	Halle, GE, Germany	Metabolomics Society
Metabolomics Engineer	MetaCom, Institute for Plant Biochemistry	Halle, GE, Germany	Metabolomics Society
Technical Core Director for LC/MS/MS, IRMS, and GMCS analyses	UT Health San Antonio	San Antonio, TX, USA	UT Health San Antonio
Post-Doc Fellowship in Cancer Epidemiology	American Cancer Society	Atlanta, GA, USA	American Cancer Society
Laboratory Technician in Metabolomics	The Molecular Discovery Platform at CeMM	Vienna, Austria	<u>CeMM</u>
Scientific Analyst	University of Arizona	Tucson, AZ, USA	University of Arizona
Scientist, Research Data	University of Arizona	Tucson, AZ, USA	University of Arizona
Post Doctoral Position in Human Nutrition:	The French National Research Institute for	France	INRAE

Metabolomics-based exploration

Agriculture, Food, and the Environment (INRAE)

Postdoctoral Fellow –
Microsampling devices for
lipidomics

Concordia University

Montreal, QC, Canada The Metabolomics
Innovation Centre
(TMIC)

# **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 <a href="mailto:metabolomics.innovation@gmail.com">metabolomics.innovation@gmail.com</a>

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