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**The MetaboNews Team**

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

## Metabolomics Society News

### **Board of Directors**

Dear Colleagues,

What an amazing event we had in Valencia! It was such a treat to see so many colleagues and to share our research in person! We certainly had an incredible time being together. We have a brief update on the conference in this edition of MetaboNews, but will expand upon this in an upcoming issue. For those of you taking some time off for the summer, I hope that you are enjoying a much needed break. There are a couple brief updates that I would like to highlight for you on how you may get more involved with the Society this year:

- Please consider running for the Board of Directors of the Metabolomics Society. Nominations should be submitted by July 30. There are 12 open positions this year. Keep an eye out for the email announcing the Call for Nominations.
- We also have new positions for the Early-career Members Network (EMN). If you are an early-career member, please consider running for one of these positions. You won't regret it, as this is one of the most active parts of our Society.

Enjoy the summer!

All the best,

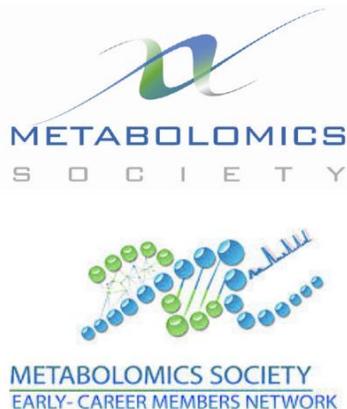


Jessica Ann Lasky-Su  
President of the Metabolomics Society



## Members' Corner

### Early-career Members Network (EMN)



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)

Are you an early-career researcher and want to join the Early-career Members Network (EMN) committee?

We welcome applications from graduate students and researchers up to 5 years after accomplishing a PhD to join one of the 8 committee positions for the next term of 2022/2023! Find out more and apply through 31st July 2022 by following the link here: [https://bit.ly/EMN\\_committee](https://bit.ly/EMN_committee)

A banner for TMIC (The Metabolomics Innovation Centre). The background is light blue with a molecular structure graphic on the right. On the left is a red logo consisting of three hexagons. The text 'TMIC The Metabolomics Innovation Centre' is in large, bold, black letters. Below it, in a smaller blue font, is 'Comprehensive metabolomics and lipidomics services'. There are four icons in hexagonal frames: a bar chart, a network diagram, a computer monitor with a graph, and a multi-omics diagram. Each icon is followed by text: 'Quantitative metabolomics services', 'Global metabolomics &amp; lipidomics profiling', 'Customized assay development', and 'Bioinformatics services'. At the bottom, there is a red circle with a white envelope icon and the email 'info@metabolomicscentre.ca'. To the right is a QR code with a hand pointing to it and the text 'SCAN ME'. At the bottom center are the LinkedIn and Twitter social media icons.

## International Affiliates' Corner

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

Visit <http://lamps-network.org>

The LAMPS founding members are delighted to invite you to the **IV LAMPS meeting**, which will be held in Cartagena, Colombia, on November 2-4, 2022. The meeting will take place at Universidad de los Andes - Sede Caribe, which is located in the Serena del Mar urban development at 12 km from the historic centre of Cartagena (<https://caribe.uniandes.edu.co/es>). This is the first time that the LAMPS meeting will be held in Colombia, and our first in-person meeting after postponing it for two years due to the COVID-19 pandemic. The LAMPS founding members and the Organizing Committee are looking forward to seeing you all in Cartagena. More information about the conference, the list of confirmed speakers, registration, and the venue can be found at <https://live.eventtia.com/en/lamps-meeting-colombia/home>.



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

Visit <https://metabolomicsna.org>

#### **4th Annual MANA Conference**

The [4th Annual MANA Conference](#) will be held **September 16-18, 2022, in Edmonton, Alberta, Canada**. We very much look forward to welcoming you in a couple months, and hope that you are equally excited to return to in-person discussions of the latest science and technology developments in the field of metabolomics.

	<b>Registration Fees</b>
<b>Regular (non-trainee) Fees</b>	\$375.00 USD
<b>Early Career Member Fees</b>	\$325.00 USD

### **Conference abstract deadlines extended**

Poster abstracts July 22, 2022, 4 pm PT

The conference Instructional Workshops and Interactive Forums have been finalized in the program and are as follows:

#### **Instructional Workshops**

##### **☐ Friday, September 16, 2022**

- MetaboAnalyst - Prof. Jeff Xia, McGill University
- Frontiers in NMR Metabolomics - Prof. Leo Cheng, Harvard Medical School and MANA NMR Interest Group
- How Do We Best Teach Metabolomics? - Dr. Arpana Vaniya, UC Davis and MANA Educational Resources Committee

##### **☐ Saturday, September 17, 2022**

- Metabolomics Workbench and the National Metabolomics Data Repository - Dr. Eoin Fahy, UC San Diego

##### **☐ Sunday, September 18, 2022**

- National Microbiome Data Collaborative: Metabolomics Data Processing Workflows and Metadata Standards - Ms. Montana Smith & Dr. Yuri Corilo, PNNL; Dr. Chris Mungall, LBNL

#### **Interactive Forums**

##### **☐ Friday, September 16, 2022**

- Precision Medicine Discipline - Prof. Rima Kaddurah-Daouk, Duke University and MANA Precision Medicine Interest Group
- Wine- and Beer-Tasting for Metabolomics - Prof. David Wishart, University of Alberta and TMIC

##### **☐ Saturday, September 17, 2022**

- Urgent Issues in NMR - Dr. Tracey Schock, NIST and MANA NMR Interest Group
- NIST Development of a Fecal Metabolite Calibrant - Dr. Sandra Da Silva, NIST
- Software and Data Exchange (SODA) - Dr. Ewy Mathé, NIH and MANA SODA Interest Group

#### **Plenary Sessions**

[Plenary speakers](#) include Dr. Philip Britz-McKibbin, Dr. Yamilé López Hernández, Dr. Russell Jones, Dr. Laura-Isobel McCall, Dr. Nadja Cech, and Ms. Kathryn McCauley, MPH. Check the [conference website](#) for continued updates to the conference program.

### **MANA SODA Interest Group**

Join us for our next MANA SODA Meet on Tuesday, August 9th at 3pm ET! Our speakers will be our new SODA Co-lead, Daniel Hitchcock (Broad Institute), and Andy Patt (NCATS/NIH). 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. To get involved and to learn more, visit our [SODA webpage!](#) If you're interested in presenting a tool, data, or idea, in any stage of development please reach out to [soda-committee@metabolomicsna.org](mailto:soda-committee@metabolomicsna.org).

### **Swiss Metabolomics Society (SMS)**

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

The **Swiss Metabolomics Society Meeting 2022** will

take place on September 29th in Lausanne! A great line-up of speakers, including **Oscar Yanes** (Universitat Rovira i Virgili, Tarragona, Spain), **Martin Giera** (Leiden University Medical Center, Netherlands), **Fabien Jourdan** (INRAE, Toulouse, France), and **Mojgan Masoodi** (Bern University Hospital, Bern, Switzerland), will talk about the latest advancements in metabolome annotation and data interpretation in a biologically relevant context and the application of metabolic phenotyping in clinical research (from patient stratification to treatment strategies). The Meeting will be followed by an After-Meeting School "From data to biologically relevant information" on September 30th, with Oscar Yanes, Martin Giera, Julien Boccard, and Fabien Jourdan as instructors. For registration and detailed program, please visit <https://swiss-metabolomics.ch/annual-meeting/>. The number of participants is limited.

# MANA 2022

## September 16-18, 2022 - Edmonton, Alberta, Canada

### **Plenary Speakers**

- Dr. Philip Britz-McKibbin
- Dr. Nadja Cech
- Dr. Russell Jones
- Dr. Yamilé López Hernández
- Dr. Laura-Isobel McCall
- Kathryn McCauley, MPH

[Workshops](#)

[Networking](#)

[Awards](#)

[Events](#)

### **Registration is open!**

**Revised Deadlines**  
Poster Abstracts – July 22  
Childcare Grants – July 22

Check [MANA2022.net](http://MANA2022.net)  
for themes

We are pleased to present this special edition of MetaboInterview! Get to know the 2022 award recipients who were announced at this year's Metabolomics Society conference in Valencia, Spain.

- Honorary Fellowships:
  - Prof. Lorraine Brennan
  - Prof. David Broadhurst
- Metabolomics Society Medal: Dr. María Eugenia Monge
- President's Award: Dr. Rachel Kelly

## Honorary Fellow of the Metabolomics Society: Lorraine Brennan, PhD



*An Honorary Fellowship is a significant lifetime award granted by the Metabolomics Society to exceptional members of the metabolomics community. Lorraine played a key role in establishing the field of nutritional metabolomics, through the identification of dietary biomarkers and the implementation of dietary interventions, moving the field toward personalized nutrition.*

Lorraine Brennan is a Full Professor in the School of Agriculture and Food Science, University College Dublin, Ireland.

### **Tell MetaboNews readers about yourself.**

I am a full professor and a PI in the Institute of Food & Health and the Conway Institute, both in University College Dublin (UCD), Ireland. My work for the development of metabolomics-based approaches for improvements in dietary assessment was recognized by a European Research Council (ERC) Consolidator Grant award. Currently I am involved in a number of

European consortia including PROMED-COG and PlantIntake.

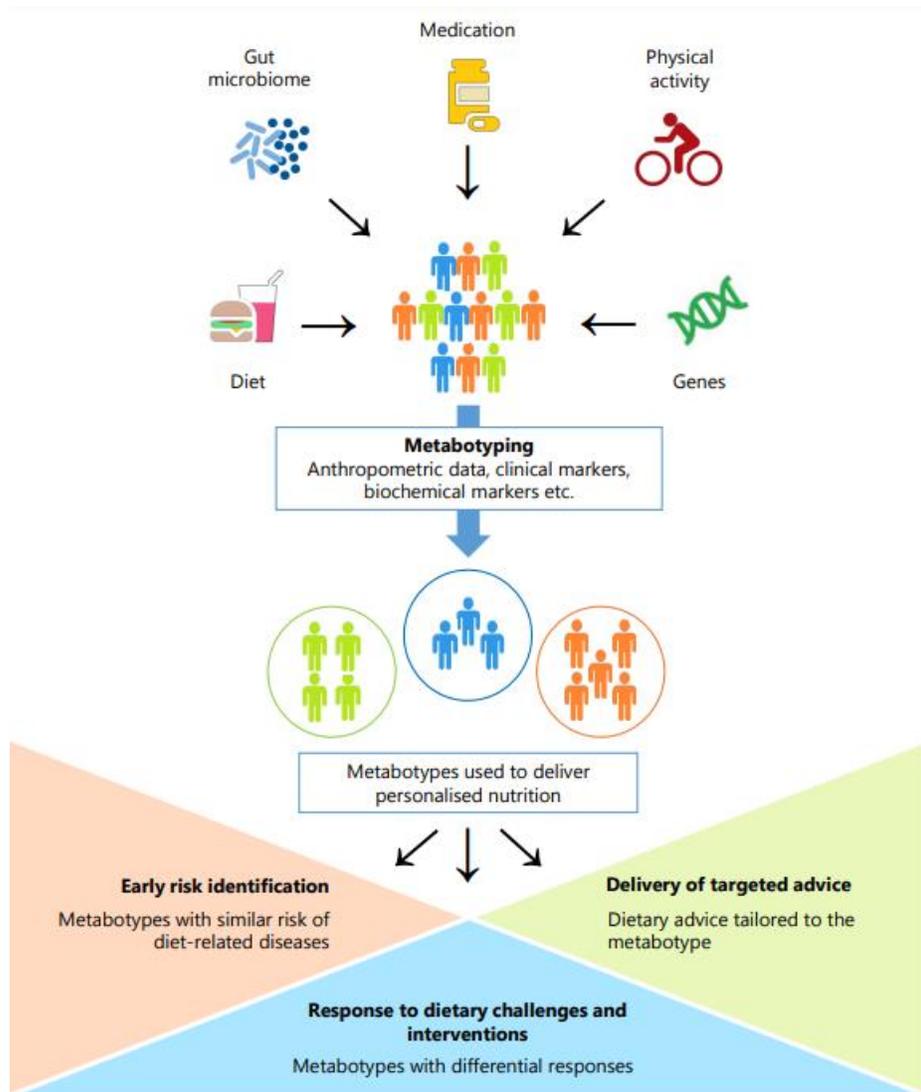
I served as Director of the European Nutrigenomics Organisation for 5 years and led a number of important initiatives such as the development of an Early Career Network and expansion of membership of the organization. Recently, I was appointed to the (US) National Academies of Science, Engineering, and Medicine Standing Committee on Evidence Synthesis and Communications in Diet and Chronic Disease Relationships.

Also, I am involved in a number of public outreach activities and I edit the Frontiers for Young Minds special collection: New ways to understand how foods affect me and my health.

**What are the highlights of your current metabolomics research?**

Examples of current highlights from our research include (1) development of dietary biomarkers and (2) development of approaches to deliver personalized nutrition advice.

Accurate assessment of what people eat remains a key challenge in nutrition research and dietary biomarkers offer the potential of obtaining objective measures of intake. Our work in the field has been instrumental in showing how one can use these biomarkers to estimate intake of certain foods. The significance of this study lies with the fact that it clearly demonstrates how biomarkers may be used in a larger cohort/population setting to estimate food intake. Additionally, we have developed statistical tools and software for dietary biomarkers (<https://www.ucdnutrimarkers.com/software>).



**Figure 1:** Overview of the concept of metabotyping for the delivery of personalised nutrition. Intrinsic and extrinsic factors influence the metabolic phenotype of individuals. Groups of individuals with similar metabolic phenotypes are termed metabotypes. (Graphic taken from [Nutr Res Rev. 33, 33 \(2019\).](#))

With respect to Personalized Nutrition there is now an acceptance that there is a need to move away from “one size fits all” guidelines to a more personalized approach. Work in our group in this field has focussed on the concept of “metabotypes” and tailoring of nutrition advice to different metabotypes. In particular, we have developed a framework where a metabotyping approach could be used to deliver targeted nutrition advice to a population group.

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

Dietary biomarkers have great potential in the Nutrition research area. Using biomarkers, it is possible to obtain information on food intake and it can help address some of the measurement errors associated with the classical self-report methods. This in turn will improve the accuracy of dietary assessment and provide a complementary tool to traditional dietary assessment methods. Combining biomarkers with classical approaches offers the potential to capture the full dietary intake with

improved accuracy. Another area where metabolomics-based biomarkers have great promise is the classification of individuals into different dietary patterns. Further work in a broader range of dietary patterns and population groups are necessary to realize the full potential. In summary, the emerging data is very exciting for the future role of biomarkers of food intake. While many putative biomarkers now exist, there is an urgent need to validate these biomarkers so that they can be used in nutritional epidemiology. The validation steps require rigorous assessment of the performance of the biomarkers including their stability, reproducibility, time-response, and dose-response. Looking to the future I

hope that fully-validated biomarkers will exist for many foods, allowing a comprehensive and accurate assessment of food intake.

With respect to Personalized/Precision Nutrition, metabolomics is set to play a key role. The concept of using a metabotype approach to tailor advice to groups of metabolically similar individuals is expanding beyond the nutrition field. Many studies have now reported metabolite sub-clusters in individuals with type 2 diabetes and there is an expectation that lifestyle advice can be tailored to the sub-groups. Metabolomics will play a key role in the further development of these concepts.

## Honorary Fellow of the Metabolomics Society: David Broadhurst, BEng (Hons), MSc, PhD



***The Metabolomics Society Lifetime Honorary Fellowship is a significant award granted to exceptional members of the metabolomics community. It recognizes making a pioneering and sustained contribution to the science of metabolomics at an international level, within the fields of technology development, computational biology or application to a specific discipline. It also recognizes any outstanding contributions to the Metabolomics Society over a sustained period of time.***

David Broadhurst is the Professor of Data Science & Biostatistics and Director of the Centre for Integrative Metabolomics & Computational Biology at Edith Cowan University, Australia.

### **Tell MetaboNews readers about yourself.**

I hold a first-class honours degree in Electronic Engineering, an MSc in Medical Informatics & Instrumentation, and a PhD (1997) in the “Application of Artificial Neural Networks and

Evolutionary Computation to Chemometric Data Analysis”. I started my professional academic career at Aberystwyth University (Wales) during the inception of both Systems Biology and Metabolomics. I worked under the guidance of Professors Douglas Kell and Royston Goodacre. In 2004, I relocated to

the University of Manchester (UK) as a postdoctoral research fellow, where alongside Warwick Dunn I helped advance the use of untargeted mass-spectrometry metabolic profiling in understanding human pathology. In 2009, I moved to the Department of Obstetrics and Gynaecology, University College Cork, Ireland, where, alongside Professor Louise Kenny, I was instrumental in the foundation of pregnancy-related metabolomics with particular emphasis on discovering early-onset metabolite biomarkers for pregnancy complications. In 2011, I moved to the University of Alberta, Canada, where I was appointed Assistant Professor of Biostatistics and lead scientist for the Faculty of Medicine's Clinical Metabolomics, working closely with Professor David Wishart (Faculty of Science) and Professor Brian Sykes at the National High Field Nuclear Magnetic Resonance Centre (NANUC). In March 2016, I was recruited to Edith Cowan University (ECU) as part of a strategic government initiative to enhance clinical metabolomics and systems biology capabilities in Western Australia. I was given the opportunity to establish a more personal project in the form of the proof-of-concept Centre for Integrative Metabolomics and Computational Biology (CIMCB).

### What are the highlights of your current metabolomics research?

I have been an active member of the metabolomics community since completing my PhD in 1997. Throughout my career, I have been a strong advocate for statistical best practice in the metabolomics community. In 2006, I published my first position paper with Prof. Douglas Kell, "[Statistical strategies for avoiding false discoveries in metabolomics and related experiments](#)", which was well received by the community and widely cited ever since. In 2007, I co-led a working group with Roy Goodacre to establish the "[Proposed minimum reporting standards for data analysis in metabolomics](#)", which has been adopted by the Metabolomics Society and the *Metabolomics* journal. Starting in 2011, my advocacy for methodological best practice led to my most defining contributions to the field. I was a member of the

HUSERMET consortium, which aimed to define the healthy human serum metabolome in the UK population. I developed the design-of-experiments protocol, the batched analytical design principles, and computational metabolomics workflows from raw data to data cleaning and curation; these processes formed an integral component of the [2011 Nature Protocols paper](#) that has become the gold standard for clinical mass spectrometry-based metabolomics studies. This study acted as a springboard for me, Warwick Dunn, Ian Wilson and Andrew Nicholls to establish the gold standard methodology for QA/QC which has become ubiquitously adopted in the field. From the publication of the first papers (ca. 2012), I have travelled extensively to promote the use of QA/QC procedures. In 2018, I led the QA/QC guidelines paper. More recently, I have redoubled my research in Data Science, promoting FAIR (findability, accessibility, interoperability, and reusability) and Open Access best practices for statistics and machine learning. My team has won the journal *Metabolomics* best publication award three years in a row (2019-2021).

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

My current and future work will primarily focus on transforming the theoretical best practices in QA/QC, statistics, data science and machine learning, into computational tools accessible to as wide an audience as possible. A major concern I have with current trends in computational metabolomics is that software is being developed by computer scientists for computer scientists. Having open access code (R, Python, MATLAB, etc.) is incredibly important for the future of our science; however, I feel the emphasis on openness has taken precedent over usability and understanding. This often results in non-computational researchers blindly running scripts back-to-back with no real understanding of the underlying algorithms or parameter settings and praying that the resulting data is usable. This intellectual dissonance places a huge cognitive load on biological/analytical researchers/students. They are

expected to educate themselves to be competent computer scientists often at the same time as understanding complex statistical/analytical concepts. I believe that concepts first need to be taught outside of the programming domain. Only then should practitioners be exposed to the terrors of trying to successfully install and run R packages.

The first product of this project is the development of a desktop app as a companion to our [2018 QA/QC guidelines paper \(Metabolomics, 14, art 72 \(2018\)\)](#). It illustrates the process of within- and between-batch correction (based on pooled QC samples), and

interactively allows users to filter peaks on a number of quality criteria. This data-cleaning process is presented graphically via several data visualization methods (see figure below). Although designed fundamentally with education at the forefront, this software can also be used as a serious research tool (the software is currently undergoing beta testing). The aim of this and future software tools from my lab is to encourage researchers to look at their data. Metabolomics is not just about blindly applying dogmatic rules (e.g.,  $p < 0.05$  or  $RSD < 20\%$ ) but about understanding and applying concepts fit-for-purpose.

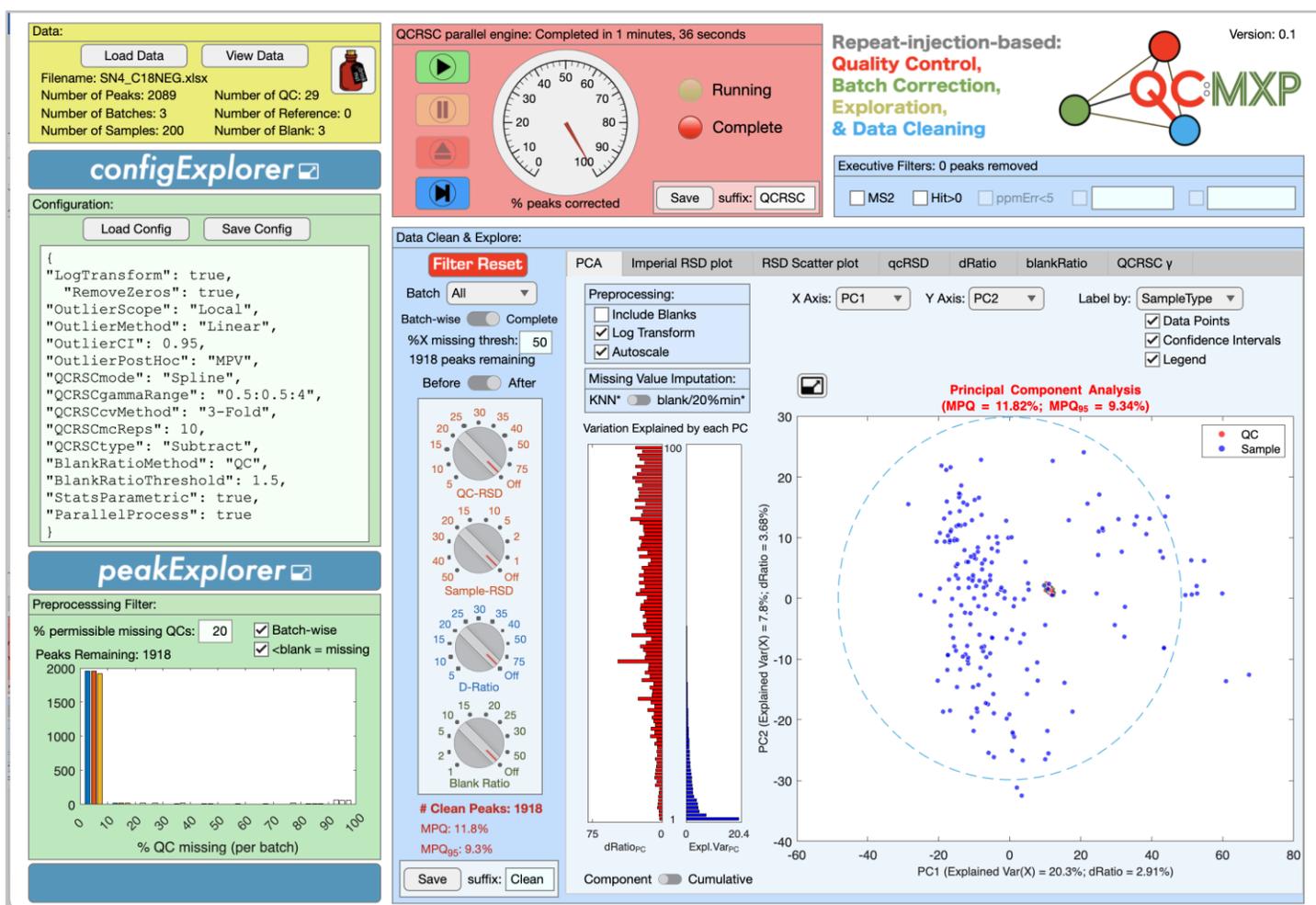


Figure 2: Visualization of data-cleaning process in desktop app being developed.

## Metabolomics Society Medal: María Eugenia Monge, PhD



*The Metabolomics Society Medal is for mid-career members of the Society and is open to those members who have been awarded a PhD 10-15 years prior to the nomination.*

María Eugenia Monge is an Independent Researcher of CONICET, the National Scientific and Technical Research Council of Argentina.

### Tell MetaboNews readers about yourself.

I am an Independent Researcher of CONICET and work at the *Centro de Investigaciones en Bionanociencias* (CIBION). In 2006, I obtained my PhD in analytical and physical chemistry from the University of Buenos Aires. Between 2007 and 2014, I held postdoctoral positions

in Italy, France, and the USA. In 2014, I was recruited by CONICET to set up a new laboratory in a new research centre and start a research group in a scientific area that was new in Argentina. I lead the Bioanalytical Mass Spectrometry Group and the Mass Spectrometry facility of CIBION (<https://cibion.conicet.gov.ar/mass-spectrometry/?lan=en>). My research group develops



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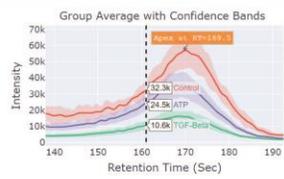
Sample extraction and collection  
*(ex. Sample 1, 2, ..., N)*



Data collection by LC-MS



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**Questions?**  
Do you have questions about your metabolomics data? Let's talk!

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  [contact@biorankings.com](mailto:contact@biorankings.com)  
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MS-based analytical methods using metabolomics and lipidomics approaches with applications in health and the environment. I am co-author of 49 peer-reviewed publications (<https://orcid.org/0000-0001-6517-5301>). I have coordinated metabolomics courses for South American students and have participated in strengthening our scientific community. Since 2021, I am a founding member of the Latin American Metabolic Profiling Society or LAMPS ([www.lamps-network.org](http://www.lamps-network.org)). Since 2019, I have been a member of the Metabolomics Society, where I serve on the Membership Committee; and I am a member of the Metabolomics Quality Assurance & Quality Control Consortium (mQACC). I also served as guest editor for the journal *Metabolites*, and I am an editorial board member of *GigaByte*.

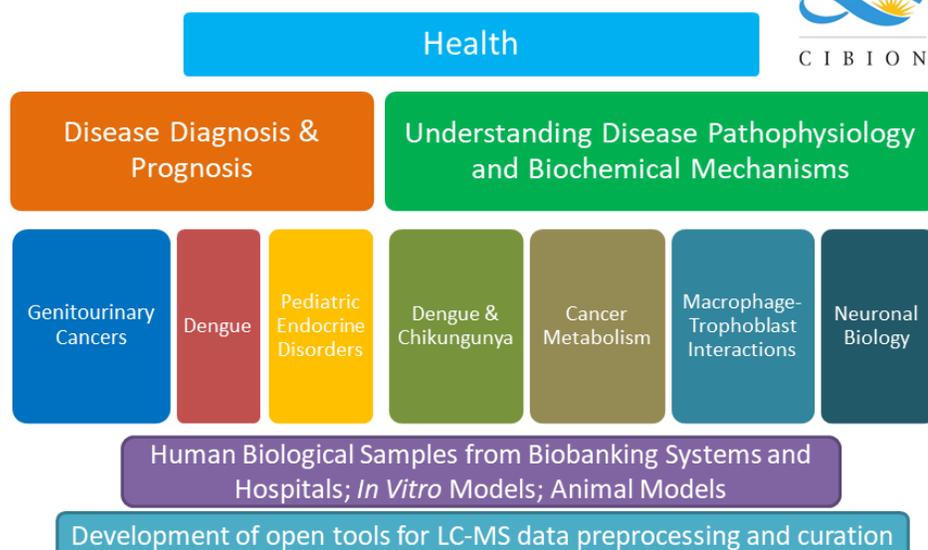
**What are the highlights of your current metabolomics research?**

One of the goals of my research group is to develop alternative analytical strategies to improve the performance of existing diagnosis and prognosis methods that are currently implemented in the clinics and to understand altered pathways in disease progression. Our initial untargeted metabolomics efforts focused on clear cell renal cell carcinoma (ccRCC) biomarker discovery and the understanding of disease physiopathology. Findings from my group

provided a proof of concept that conditioned media can be used as a serum proxy to obtain disease-related metabolic signatures; and we validated results from metabolic profiling experiments targeting the endometabolome of *in vitro* models with biological and bioinformatics assays. In addition, we obtained lipid panels for ccRCC detection and early diagnosis through an untargeted serum lipidomics-machine learning strategy. Based on these results, we are currently exploring new high-throughput analytical methods for ccRCC detection. Another ongoing project is ocused on improving prostate cancer detection by evaluating findings from previous biomarker discovery studies on an Argentine cohort. My team also develops quantitative targeted assays to contribute to the diagnosis of pediatric endocrine disorders. With the workflows and procedures developed in my group, we have expanded into other untargeted and semi-targeted metabolomics collaborations with several colleagues, and we are moving beyond biomarker discovery toward the understanding of biochemical mechanisms to answer different biological questions. In this sense, we are applying pharmacometabolomics strategies for assessing new antivirals for dengue and chikungunya; and we aim to enhance our understanding of dengue biology in the South American population, where the disease is endemic. In a different interdisciplinary project, we are in search of the neuronal metabolome

by investigating the effect of different stimuli on neurons from animal models to extend results to different models of the nervous system. In addition, my group collaborates to investigate the metabolic reprogramming of macrophages induced by macrophage-trophoblast interactions during the early stages of gestation. Furthermore, my research group is continuously updating capabilities of TidyMS, a Python-based package for preprocessing LC-MS data for quality control procedures in untargeted metabolomics workflows.

Multidisciplinary Research Projects of the Monge Group



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

I see my work in metabolomics as a powerful tool to improve our current understanding of alterations in metabolic pathways in living organisms and models; to connect the phenotypes with health and disease statuses; to contribute to drug discovery; and to improve clinical readouts. My work has also provided tools to bridge marine and atmospheric chemistry, which directly impact air quality, climate change, and human health ([Atmos Chem Phys, 20, 6243 \(2020\)](#)).

In the future, I believe that metabolite panels are promising in translating metabolomics findings into the clinical setting under the shape of diagnostic tests, changing the current diagnosis paradigm. In particular, ambient and direct to MS-based methods have the

potential to provide a molecular diagnosis alternative to be implemented in the clinic worldwide through the coupling with machine learning methods.

I also think that technologies will be faster and more affordable for their use *in situ*, contributing to global health equity. In addition, I believe that more international collaborative efforts will be conducted to validate results among different laboratories through consent quality control practices, promoting the advancement of this field.

Finally, I am optimistic about the future scenario in South America, where I envision a growth in the field, larger access to technological developments and therefore, future contributions from this geographical area. In this regard, I believe that collaborative initiatives will lead to win-win opportunities.

## President's Award Recipient: Rachel Kelly, PhD



***The President's Award recognizes outstanding achievements in metabolomics. It is available for Society members who have been awarded a PhD no more than 5-10 years prior to the nomination.***

Rachel Kelly is the Assistant Professor of Medicine and Associate Epidemiologist at the Channing Division of Network Medicine (CDNM), Department of Medicine at Brigham and Women's Hospital and Harvard Medical School, Boston, USA.

### Tell MetaboNews readers about yourself.

I am an Assistant Professor of Medicine and Associate Epidemiologist at the Channing Division of Network Medicine (CDNM), Department of Medicine at Brigham and Women's Hospital and Harvard Medical School in Boston. My work primarily focusses on the use of metabolomic epidemiology studies as a means

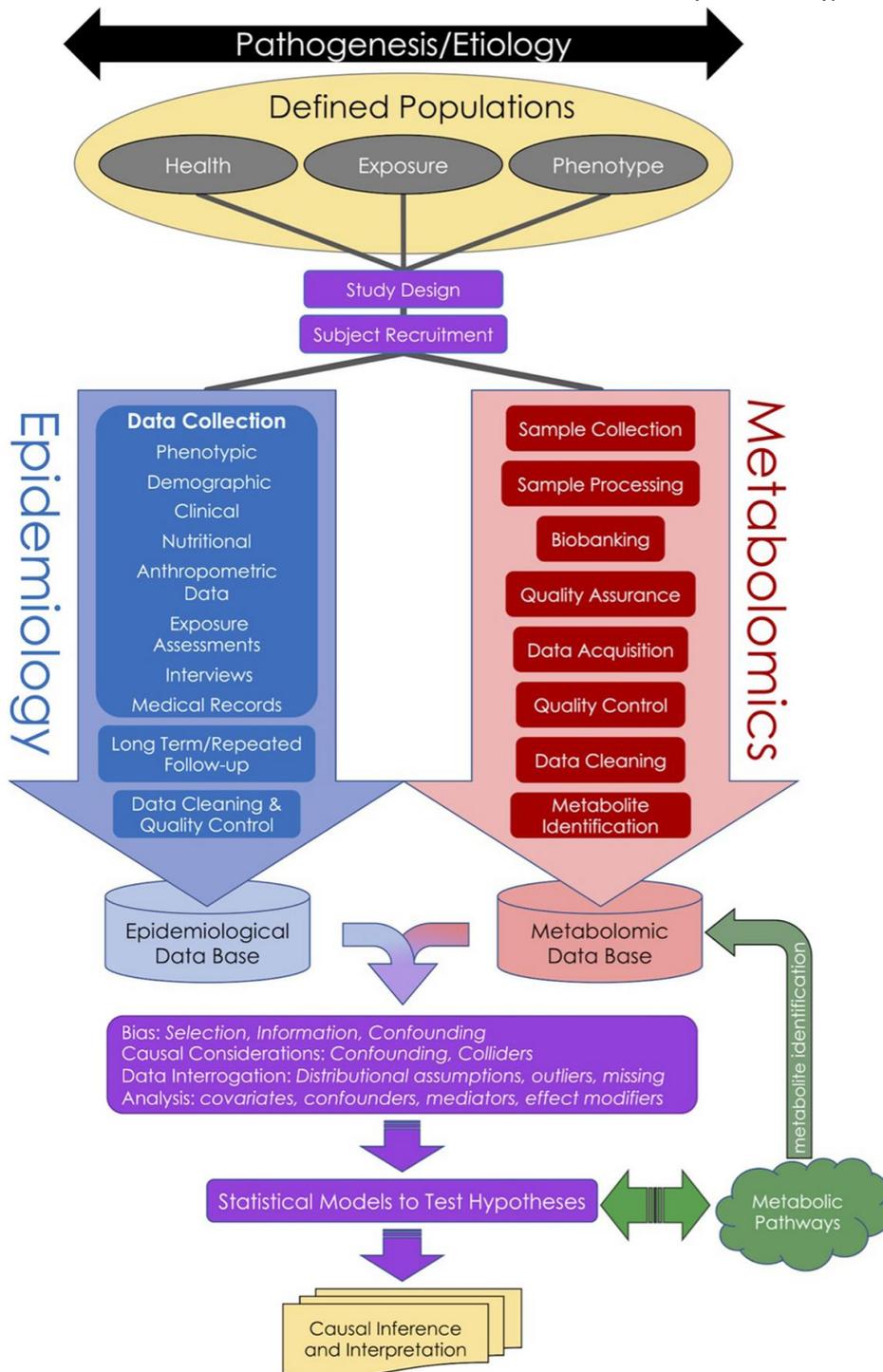
to better understand complex chronic disease. I was introduced to metabolomics during my graduate work at Imperial College London which was aimed at the identification of molecular, genetic and -omic biomarkers of non-Hodgkin Lymphoma (NHL). I then undertook two postdoctoral fellowships at the Harvard TH Chan School of Public Health and at the CDNM where I developed my graduate work to focus

on the integration of multiple -omic platforms using network theory approaches to better understand lung health. Now at faculty level, my primary research involves the integration of metabolomic data with other -omic data and clinical biomarkers to study early life health and development.

**What are the highlights of your current metabolomics research?**

The concept I am most excited about right now is the derivation of metabolomic-driven disease endotypes (subtypes defined by a distinct functional or pathobiological mechanism), which may help to

improve the treatment or management of disease by targeting the specific biology of a given subgroup. Metabolomics reflects genetics, environmental factors, and their interactions, and as the 'ome closest to phenotype, it provides insight into the physiological state of an individual. As such, it represents a particularly compelling approach to the identification of endotypes. I demonstrated this in asthma, a highly heterogenous disease where I was able to derive and, crucially, validate five metabolomic endotypes with clinically relevant differences in lung function using two independent cohorts of children with asthma ([Am J Respir Crit Care Med, 205, 288 \(2022\)](#)). Interrogation of the metabolites driving these endotypes revealed differences in pathways relating to pulmonary surfactant homeostasis, a critical component of lung function. In this paper I coined the term "metabo-endotype" and our lab is currently working to derive metabo-endotypes of other heterogenous disorders including Autism Spectrum Disorder and Age-Related Macular Degeneration; and to integrate additional -omic data types into these analyses.



**Figure 3:** Graphical representation of the components and typical workflow for Metabolomic Epidemiology.

Outside of my primary research, I am passionate about advancing the overall field of metabolomic epidemiology. I serve on the Metabolomic Epidemiology Task Force of the Society, and we are working to ensure the growth of this field and to address the accompanying challenges ([Metabolomics, 17, 45 \(2021\)](#)). In my opinion, one of the biggest developments in metabolomic epidemiology is the establishment of The Consortium Of METabolomics Studies (COMETS) ([Am J Epidemiol, 188, 991 \(2019\)](#); [191, 147 \(2022\)](#)) which now includes over 80 prospective metabolomics cohorts, and >150,000 participants from all over the world. I serve on the executive committee of COMETS and am leading one of the first twometabolomic meta-analyses, seeking to identify BMI-associated metabolites in the largest metabolomic study of BMI ever conducted. I am excited to soon publish this work and to help others navigate the complexities of large scale metabolomic epidemiology meta-analyses within the COMETS framework.

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

For me the ultimate achievement would be helping to make a tangible difference in people's health. Although the derivation of asthma metabo-endotypes represents just the first step in translation to the clinic, I do believe they provide strong candidates for more precise and personalized asthma management strategies while informing on underlying mechanisms. As we continue to explore metabo-endotypes of other conditions, we hope to see equally promising results.

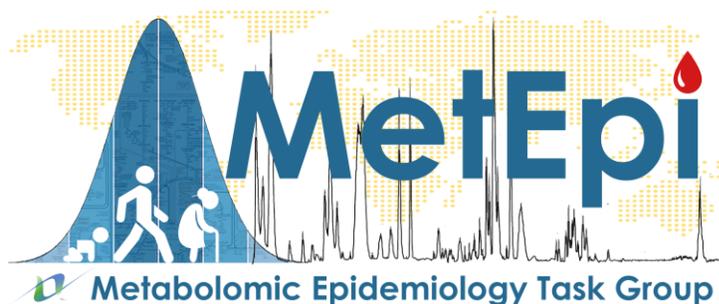
Similarly, I am interested in maternal health in pregnancy and its impact on the health of offspring ([Metabolites, 11, 65 \(2021\)](#)). I am currently leading two projects within the National Institutes of Health Environmental Influences on Child Health Outcomes (ECHO) program, exploring the links between the maternal metabolome and childhood obesity and neurodevelopment within five mother-child cohorts. I am hoping with these results we can leverage the ways

in which the metabolome informs on environment and its modifiable nature to discover novel means of improving the prenatal environment and ultimately child health.

More generally in the field, I see COMETS, and particularly software they have developed to streamline consortia meta-analysis, as a game changer (<https://www.comets-analytics.org>; [Am J Epidemiol, 191, 147 \(2022\)](#)). I am co-leading the COMETS lung interest group, and the goal of this group is to conduct simultaneous meta-analyses of 13 different lung phenotypes across 160 different models to generate the mostcomprehensive understanding of lung metabolomics to date. This work is being led by 20 PIs working together to develop these models and to interpret their results and represents a new paradigm in efficiently and effectively conducting consortium-based research.

I also hope that my work to develop an extension of the STROBE reporting guidelines specifically for metabolomic epidemiology with a team of international experts (<https://www.equator-network.org/library/reporting-guidelines-under-development/reporting-guidelines-under-development-for-observational-studies/#MetEp>), will be embraced by both the community and by relevant journals. By developing a consensus for how metabolomic epidemiology studies should be reported, we can strengthen both the science and the field as a whole.

Overall, I think it's such an exciting time to be working in metabolomics and I can't wait to see what the next ten years hold!



## Recent Publications

### Recently published papers in metabolomics

- [A multi-omics analysis for the prediction of neurocognitive disorders risk among the elderly in Macao](#) (Open access)
- [Acylcarnitines: Nomenclature, Biomarkers, Therapeutic Potential, Drug Targets, and Clinical Trials](#) (Review, Open access)
- [Analytical aspects of meet-in-metabolite analysis for molecular pathway reconstitution from exposure to adverse outcome](#)
- [ATF4 Protects the Heart From Failure by Antagonizing Oxidative Stress](#)
- [Combined nature and human selections reshaped peach fruit metabolome](#) (Open access)
- [Comparative physiological and metabolomic analyses reveal that Fe<sub>3</sub>O<sub>4</sub> and ZnO nanoparticles alleviate Cd toxicity in tobacco](#) (Open access)
- [Effects of polyethylene and polylactic acid microplastics on plant growth and bacterial community in the soil](#)
- [Fibroblasts Drive Metabolic Reprogramming in Pacemaker Cardiomyocytes](#) (Open access)
- [High-throughput plant phenotyping: a role for metabolomics?](#) (Review, Open access)
- [Measuring biological age using omics data](#) (Review)
- [Metabolic regulation of prostate cancer heterogeneity and plasticity](#)
- [Multiomics analyses uncover nanoceria triggered oxidative injury and nutrient imbalance in earthworm \*Eisenia fetida\*](#)
- [Sensor-based MIP technologies for targeted metabolomics analysis](#) (Open access)
- [Understanding the role of biochar in affecting BDE-47 biodegradation by \*Pseudomonas plecoglossicida\*: An integrated analysis using chemical, biological, and metabolomic approaches](#)
- [Using MetaboAnalyst 5.0 for LC-HRMS spectra processing, multi-omics integration and covariate adjustment of global metabolomics data](#) (Protocol extension, Open access)



# Metabolomics Events

**May 29-June 2, 2022**

19th International GCxGC Symposium

Venue: Online

[Learn More Here](#)

## Overview

While we had planned to host the meeting in beautiful Canmore, Alberta, Canada, we are now moving to a fully virtual event. The technical program includes the 2022 John B. Phillips and Scientific Achievement Award Lectures, 3.5 full days of live talks, posters and discussion sessions, and opportunities to contribute virtual talks and posters.

Update: We held the conference already but you can still access the conference platform until September 2. Registration is open whether or not you attended the meeting.

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**July 25, 2022**

Pre-Application Webinar for NCI's Technologies and Informatics Tools for Cancer Metabolomics NOSI (NOT-CA-22-083)

Venue: Online

[Learn More Here](#)

## Overview

NCI will hold a pre-application webinar on Monday, July 25, 2022, from 1:00 p.m. – 2:00 p.m. (EDT) for the Notice of Special Interest (NOSI) NOT-CA-22-083, "Notice of Special Interest (NOSI): Technologies and Informatics Tools for Cancer Metabolomics."

This pre-application webinar will be focused on NCI's interest in metabolomics technologies and informatics tools and overviews of the IMAT and ITCR programs. NCI staff involved in these funding opportunities will explain the goals and objectives of the programs and answer questions from webinar attendees.

## August 5, 2022

### MANA Early-Career Members (ECM) Virtual Job Fair

Venue: Online

[Learn More Here](#)

#### Overview

Hiring new members? Looking for a new position? Gathering information for the next step in your career? Join the ECM Virtual Job Fair!

As an employer or recruiter, you'll get the opportunity to meet potential candidates. As someone who is in the market, this is a great opportunity for you to meet potential employers from different tracks (i.e., Academia, Industry, or Government/Nonprofit). We will help employers and potential candidates meet effortlessly in a virtual capacity via Zoom! Using Breakout Rooms, we'll set up and manage interviews and/or informal meetings.

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## August 9, 2022

### MANA SODAMeet

Venue: Online

[Learn More Here](#)

#### Overview

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), we will have two speakers present on software or data they would like to share with the community, emphasizing how these software/data are used.

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## August 22-September 2, 2022

### International Summer Sessions in Metabolomics

Venue: Online or Davis, California, USA (Hybrid)

[Learn More Here](#)

#### Overview

This course at UC Davis has been completely redesigned for a hybrid format and will also be recorded for the participants to view at a later time. All software training has transitioned to a virtual machine environment so training can be done from any location. Virtual machines are hosted by Amazon Web Services and can be accessed using either a PC or a Mac computer. Every unit is taught using interactive tools such as polling, using the annotation tool, utilizing non-verbal feedback, live questions, and group work.

## September 6-9, 2022

### The 2<sup>nd</sup> Nordic Metabolomics Conference (2022)

Venue: Copenhagen, Denmark

[Learn More Here](#)

#### Overview

The conference aims to highlight and discuss the latest metabolomics research in the Nordic countries and abroad, and we are proud to present an outstanding scientific program. The meeting will start with a session dedicated to early-career scientists, followed by an opening keynote lecture and a welcome reception at Copenhagen Town Hall. We have invited outstanding speakers from Europe including the Nordic countries. The meeting will also host a panel debate and a session dedicated to our sponsors. The majority of talks will be based on submitted abstracts. The deadline for registration is **August 8**.

## September 8-9, 2022

### Bits & Bites #7: Identification of unknown compounds in untargeted metabolomics using freely available software

Venue: Online

[Learn More Here](#)

#### Overview

This 10-part short course series will feature in-depth topics in untargeted metabolomics such as Bayesian statistics, a deeper look into MS-DIAL, fundamental courses in mass spectrometry, lipidomics, 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 approx. 4 hours. The courses will be conducted in a highly interactive manner, with the use of freely available software and databases. The tuition is \$150 USD per Bite.

The 7<sup>th</sup> course is “Identification of unknown compounds in untargeted metabolomics using freely available software”, taught by Dr. Arpana Vaniya. Compound identification is known as the bottleneck in metabolomics. However, there are many approaches one may consider while tackling this challenge (e.g., mass spectral library search, *in silico* fragmentation tools, database searching). This short course will provide an overview of the current status of compound identification in metabolomics. Participants will learn how to use freely available *in silico* fragmentation tools MS-FINDER and SIRIUS+CSI:FingerID, and apply those skills to some unknown challenges.

In session 2, participants will continue learning additional tools and compound identification approaches. In this short course, participants will learn how to use web-based tools such as MetFrag and CFM-ID and learn how to use MassBank of North America in NIST MS Search. Participants will get a chance to practise on unknown challenges.

## September 9-10, 2022

### 2022 World Endocrine & Obesity Conference

Venue: Online (no longer hybrid)

[Learn More Here](#)

#### Overview

The 2022 World Endocrine & Obesity Conference (2022WEOC) in collaboration with Thyroid Federation International is scheduled for September 9-10, 2022. Their focus is to bring together leading experts, researchers, and clinicians to exchange and share their experiences of various treatment procedures on endocrine care and obesity. Speaker registration is due July 15.

## September 16-18, 2022

### 4th Annual MANA Conference

Venue: Edmonton, Alberta, Canada

[Learn More Here](#)

#### Overview

The 4<sup>th</sup> Annual Conference of the Metabolomics Association of North America (MANA) will be hosted by the University of Alberta and The Metabolomics Innovation Centre (TMIC), and the organizers have developed an engaging preliminary program. Check out the website for program information, speakers, events, registration, awards, and more. [Poster abstracts and childcare grant applications are due July 22.](#)

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## September 29-30, 2022

### Swiss Metabolomics Society Meeting 2022

Venue: Lausanne, Switzerland

[Learn More Here](#)

#### Overview

The Swiss Metabolomics Society Meeting 2022 will take place on September 29th in Lausanne! A great line-up of speakers will talk about the latest advancements in metabolome annotation and data interpretation in a biologically relevant context and the application of metabolic phenotyping in clinical research (from patient stratification to treatment strategies). The Meeting will be followed by an After-Meeting School “From data to biologically relevant information” on September 30th. The number of participants is limited. The registration deadline is September 2nd.

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## October 14, 2022

### 4<sup>th</sup> MANA Fall Symposium

Venue: Online

[Learn More Here](#)

#### Overview

The 4<sup>th</sup> Fall Symposium of the Metabolomics Association of North America is entitled “We are what we eat: Metabolomics leading the way for nutritional research”.

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## October 20-21, 2022

### 7<sup>th</sup> Gateway Symposium

Venue: Online

[Learn More Here](#)

#### Overview

The 7<sup>th</sup> Gateway Symposium at the University of Kentucky is entitled “NMR in Metabolism: New methods & applications”.

## October 24-28, 2022

[EMBO Practical Course on Metabolomics Bioinformatics for Life Scientists](#)  
Wageningen University and Research, The Netherlands

[Learn More Here](#)

### Overview

This course will provide an overview of key issues that affect metabolomics studies, handling datasets and procedures for the analysis of metabolomics data using bioinformatics tools. It will be delivered using a mixture of lectures, computer-based practical sessions and interactive discussions. The course will provide a platform for discussion of the key questions and challenges in the field of metabolomics, from study design to metabolite identification. Applications are due **September 1**.

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## October 25-27, 2022

[2nd International Diabetes and Metabolic Surgery Summit](#)

Venue: Tel Aviv, Israel

[Learn More Here](#)

### Overview

The focus of IDMSS 2022 will be the relationship between obesity and type 2 diabetes and their associated complications and the beneficial results obtainable from metabolic/bariatric surgery. The Summit will bring together many of the world experts in the fields of metabolic surgery and medicine. The range and scope of the program are a must for all clinicians caring for patients suffering from metabolic diseases.

## November 2-4, 2022

### IV LAMPS Meeting

Venue: Cartagena, Colombia

[Learn More Here](#)

#### Overview

We are delighted to invite you to the IV LAMPS meeting, which will be held in Cartagena, Colombia, on November 2-4, 2022, at the Universidad de los Andes - Sede Caribe located in the Serena del Mar urban development, 12 km from the historic centre of Cartagena. This is the first time that the LAMPS meeting will be held in Colombia and our first face-to-face meeting after two years of postponing our meeting due to the COVID-19 pandemic.

On behalf of the LAMPS Founding members and the Organizing Committee we are excited to invite you to IV LAMPS. We look forward to seeing you all in person in Cartagena.

The early-bird registration deadline is July 30.

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## November 7-11, 2022

### 14th Annual Course on Isotope Tracers in Metabolic Research

Venue: Nashville, Tennessee, USA

[Learn More Here](#)

#### Overview

The 14th Annual Isotope Tracers Course in Metabolic Research: Principles and Practice of Kinetic Analysis course registration is now open! The in-person course this year will take place in Nashville, TN, USA, from November 7 – 11, 2022. Registration deadline is **October 14** or until the course is full. We highly recommend registering for the course early. The course tends to reach capacity before the registration deadline. Scholarships are available for students and postdoctoral fellows. Submit by **September 23** to be considered.

# Metabolomics Jobs

## Jobs Offered

If you have a job to post, please email the MetaboNews team at [metabolomics.innovation@gmail.com](mailto:metabolomics.innovation@gmail.com).

Job Title	Employer	Location	Posted	Closes	Source
Research Director – In vitro Diagnostics	Metabolomic Technologies Inc.	Edmonton, Alberta, Canada	20-June-2022	Until filled	<a href="#">MetaboNews Jobs</a>
Postdoctoral Position in Metabolomics and Proteomics Data, Cardiovascular Disease	Brigham and Women's Hospital	Boston, Massachusetts, USA	17-June-2022	Until filled	<a href="#">Brigham and Women's Hospital</a>
Postdoctoral Research Fellow in Metabolomics (Diabetes)	Lund University	Lund, Sweden	15-June-2022	Until filled	<a href="#">MetaboNews Jobs</a>
Post-Doctoral Researcher in Computational Metabolomics	ETH Zurich (Institute of Molecular Systems Biology)	Zürich, Switzerland	14- June-2022	Until filled	<a href="#">ETH Zurich</a>
Senior Research Associate in Mass Spectrometry	Chan Zuckerberg Biohub	Stanford, California, USA	27-May-2022	Until filled	<a href="#">CZ Biohub</a>
Postdoctoral Research Fellow (Exometabolomics)	North Carolina State University	Raleigh, North Carolina, USA	13-May-2022	Until filled	<a href="#">North Carolina State University</a>
Senior Associate Researcher in Mass Spectrometry	Icahn School of Medicine at Mount Sinai	New York City, New York, USA	6-May-2022	Until filled	<a href="#">Icahn School of Medicine at Mount Sinai</a>
Postdoctoral Research Fellow	University of Alberta	Edmonton, Alberta, Canada	4-May-2022	Until filled	<a href="#">University of Alberta</a>
Assistant Professor in Metabolomics of Adaptive Responses	University of California, Riverside	Riverside, California, USA	15-April-2022	Until filled	<a href="#">University of California, Riverside</a>
Operations Manager (TMIC-The Metabolomics Innovation Centre)	University of Alberta	Edmonton, Alberta, Canada	14-April-2022	Until filled	<a href="#">University of Alberta</a>

## Jobs Offered

Job Title	Employer	Location	Posted	Closes	Source
Research Technician (Mass Spectrometry)	University of Alberta	Edmonton, Alberta, Canada	5-April-2022	Until filled	<a href="#">University of Alberta</a>
Postdoc in Mass Spectrometry	University of Alberta	Edmonton, Alberta, Canada	1-Mar-2022	Until filled	<a href="#">University of Alberta</a>
Postdoc in Metabolomics/ Exposomics	University of Vienna	Vienna, Austria	4-Feb-2022	Until filled	<a href="#">University of Vienna</a>
Postdoctoral Research Associate (Sumner Lab)	University of North Carolina at Chapel Hill	Kannapolis, North Carolina, USA	12-Jan-2022	Until filled	<a href="#">University of North Carolina Careers</a>
Various Positions	Various	Various (within North America)	Various	Various	<a href="#">Metabolomics Association of North America</a>

## Jobs Wanted

This section is intended for very highly-qualified individuals (e.g., lab managers, professors, directors, executives with extensive experience) who are seeking employment in metabolomics.

We encourage these individuals to submit their position requests to the MetaboNews team at [metabolomics.innovation@gmail.com](mailto:metabolomics.innovation@gmail.com). Upon review, a limited number of job submissions will be selected for publication in the Jobs Wanted section.