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## Welcome and Farewell

With this issue we bid farewell to MetaboNews editor Ian Forsythe. The Metabolomics Society and The Metabolomics Innovation Centre could not be more grateful for the past 10 years Ian has spent editing, publishing, and building the infrastructure of MetaboNews to reach an international audience.

Thank you and we wish you all the best in your future endeavors, Ian.

 You will be missed! 

We would like to welcome our new MetaboNews team who have already begun working with our contributors. We look forward to the new direction MetaboNews will take under their guidance in the coming years as they continue to create a newsletter that encourages innovation and collaboration within metabolomics and related fields.

## Metabolomics Society News

### Conference Corner

#### Metabolomics 2022: Valencia, Spain - June 19-23

The 18th Annual Conference of the Metabolomics Society will be held in Valencia, Spain, on June 19-23, 2022. Planning for the meeting is well underway with several plenary and keynote speakers already confirmed.

We are happy to announce that the Bioinformatics Hub will be back following the success of MetSoc2018 and MetSoc 2019. The idea behind it is to let bioinformaticians, biostatisticians and software tool developers meet each other and especially the users to explain how their methods and tools are working or to answer data processing and analysis specific questions.

Registrations and call for Abstracts for the conference will open soon. For more information and regular updates please visit <https://www.metabolomics2022.org/>.

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



The Metabolomics Society is an independent non-profit organisation 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)

## Members Corner

### Early-career Members Network (EMN)

#### EMN Experts Opinion

Let's begin 2022 with a new expert's opinion!

In this January edition, Professor Tim Ebbels kindly shares his work about computational metabolomics and how to apply it into real problems. He also provides advice and tips for early career members working in the field of computational metabolomics. Follow the link for the full story [https://wiki.metabolomicssociety.org/index.php/Tim\\_Ebbels](https://wiki.metabolomicssociety.org/index.php/Tim_Ebbels).

## International Affiliates Corner

### Metabolomics Association of North America (MANA)

Visit <https://metabolomicsna.org>

We are very excited to announce that the 4th Annual MANA conference will take place September 16-18, 2022 on the campus of the University of Alberta in Edmonton, Alberta, CA. The conference will be hosted by the University of Alberta and The Metabolomics Innovation Centre (TMIC), and the organizers have developed an engaging preliminary program.

We look forward to seeing you there!

**TMIC** The **Metabolomics** Innovation Centre

*Comprehensive metabolomics and lipidomics services*

- Global analysis of up to 20,000 metabolites and lipids covering most known pathways
- > 50 targeted metabolomic assays starting at \$40 per sample
- Customized assays to meet special needs
- Bioinformatics analysis
- Research collaboration

[www.metabolomicscentre.ca](http://www.metabolomicscentre.ca)  
Contact: [info@metabolomicscentre.ca](mailto:info@metabolomicscentre.ca)

The advertisement features a light blue background with molecular structures. On the left, there are five hexagonal icons: a red hexagon, a blue hexagon with a white circle, a blue hexagon with a white circle and lines, a blue hexagon with a white grid, and a blue hexagon with a white bar chart.

## Hafiz Muhammad Arshad



**Ph.D. Candidate  
University of Strathclyde  
Glasgow, UK**

### Biography

Hafiz Muhammad Arshad is a Ph.D. candidate (4th year) at the University of Strathclyde in Glasgow, United Kingdom. Before starting his Ph.D. program, he served as a lecturer in reproductive physiology and endocrinology at Bahauddin Zakariya University in Pakistan. He has made valuable contributions through teaching and research publications in his field.

### Interview Q&A

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

I was introduced to this field by my mentors and supervisors Prof. Craig W. Roberts and Dr. Gareth Westrop. However, I started to work practically in the field of metabolomics to pursue a Ph.D. through a collaborative project between the University of Porto (Portugal) and the University of Strathclyde, detailing the metabolomic profile of the maternal-fetal interface during maternal infection with *Toxoplasma gondii*. This study provided insight into how the disease of toxoplasmosis affects the developing maternal-fetal interface and particularly the developing fetus. It took me some time to understand the protocol and procedural details regarding the interpretation of data; however, I must say it is quite an exciting and novel approach that can be implemented in many fields of science. Now I am confident and excited in pursuing a lifelong career in this field.

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

First of all, metabolomic profiling of the maternal-fetal interface had never been done before using mice maternally infected with *T. gondii*, to the best of my knowledge. We used an LC-MS approach to investigate, identify, and quantify the metabolites at the maternal-fetal interface during pregnancy. We identified many metabolic changes and biomarkers which could be a therapeutic target in the future. Other than this, the discovery of different metabolic changes as the infection progresses from mother to the developing fetus and how it happens is an exciting outcome.

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

Like I said, this work appears to be the first of its kind detailing the metabolic status of the very diverse environment of pregnancy, where many phases of infection, immunity, microbiota-host interaction, and metabolism overlap and interact with each other. Based on the results obtained from this study, there are a couple of hypotheses that are very likely to be addressed in future studies to further enhance our knowledge to achieve better outcomes.

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

The interest in the field of metabolomics is growing vastly all over the world now. There are many scientists from diverse disciplines that are collaborating in research in metabolomics. The work done in my Ph.D. program is also a collaborative work done between the University of Porto in Portugal and the University of Strathclyde here in the UK. Currently, in the UK, there is much happening in the field of metabolomics, including fast-growing networks of mass spectrometry-based collaborative research groups, drug development, toxicology studies, public-private partnership projects, and industry-led research. There are many but these are just to name a few.

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

Toxoplasmosis is an infectious disease of high veterinary and medical importance, and according to epidemiological studies, it can infect as much as 50% of the human population. It is of utmost importance to evaluate the consequences of infection during pregnancy, which are still largely unknown. My current project mainly focusses on the impact of maternal infection on the maternal-fetal interface and on maternal serum. There are many metabolites and metabolic pathways observed to be disrupted during maternal infection. Those disruptions in metabolic pathways could be future targets to explore further to deal with this infectious disease. As I mentioned earlier, there are a few hypotheses generated that somebody can include in future research in this particular area of zoonotic diseases.

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

Metabolomics has the potential to increase our understanding of how different enzymes, chemicals, or other biological factors can affect the human/host health. If I have to talk about the strengths of metabolomics, there are many, but in particular, I would like to mention a few of these, such as the coupling of a global analysis followed by targeted analysis, which makes it very convenient and less time-consuming to analyze a huge set of data with a high degree of identification, quantification, and validation of the metabolomic profiles. Similarly, we can process and analyze thousands of clinical samples or any large dataset in a short period of time.

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

There are some issues within metabolomics that need to be addressed. From my point of view, one of the biggest challenges faced in metabolomics research is being able to make the true identification of different putatively-identified metabolites (within untargeted metabolomics). A single putatively-identified feature in mass spec data can actually be due to various fragments and adducts. Although there are many techniques suggested by many leading scientists to solve this issue, they ultimately need to be consistent with each other. In my view, the most reliable technique recently developed is matching of retention time (RT) of any molecule with that of a standard molecule. Although these RTs can be different in different experimental conditions, time scales, and instruments used, it is still considered by many to be the most reliable technique for valid identifications of metabolites. However, I am optimistic that some more techniques will be developed in the near future to address the issue of true identifications of metabolites.

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

Generally, science is a challenging career. Sometimes, funding is uncertain for a specific area of research, so it makes it difficult to proceed. As far as metabolomics is concerned, funding is no doubt a problem at the moment and it may remain likely in the near future. However, with metabolomics being a quickly-emerging field and many scientists rushing towards using its techniques, I don't think the situation of funding will likely be as challenging in the coming years as it is today.

### **What role can metabolomics standards play?**

Innovation is derived from creative thinking and hard work. This field has been transitioning into a mature stage now due to the innovative ideas, workflows, and research being carried out. Standardization is always an essential aspect of achieving cross-validation of any outcome between different platforms and laboratories.

Like I discussed earlier, the major bottleneck in an untargeted metabolomics spectrum is the true identification of metabolites. This can be addressed by comparison with the spectra of authentic standards. This comparison can be made regarding retention time, m/z value, and structural identities; however, it is unlikely for any one laboratory to buy all of the authentic standards for the confirmation of all the putatively-identified metabolites. In reality, a reasonable compromise is to retrospectively use authentic standards to confirm those metabolites of greatest importance and where important conclusions can be made.

### **Do you have any other comments that you wish to share about metabolomics?**

Different metabolite states are the ultimate representation of the underlying biological condition. The accurate interpretation of altered metabolites can lead us to discerning and understanding minor changes in the genome or proteome that directly affect metabolism. In this way, it allows us to evaluate the entire system. This is what makes metabolomics research so valuable.

# Recent Publications

## Recently published papers in metabolomics

- [Applications of Metabolomics to Precision Nutrition](#)
- [Enantioselective Metabolomics by Liquid Chromatography-Mass Spectrometry](#)
- [Establishment of a Prognostic Prediction and Drug Selection Model for Patients with Clear Cell Renal Cell Carcinoma by Multiomics Data Analysis](#)
- [HMDB 5.0: the Human Metabolome Database for 2022](#)
- [Inferring Early-life Host and Microbiome Functions by Mass Spectrometry-based Metaproteomics and Metabolomics](#)
- [The Integrated “Multiomics” Landscape at Peak Injury and Resolution From Alcohol-Associated Liver Disease](#)
- [Integrating \*in vitro\* Metabolomics with a 96-well High-throughput Screening Platform](#)
- [Integration of GWAS, Metabolomics, and Sensorial Analyses to Reveal Novel Metabolic Pathways Involved in Cocoa Fruity Aroma GWAS of Fruity Aroma in Theobroma cacao](#)
- [Mapping the Human Gut Mycobiome in Middle-aged and Elderly Adults: Multiomics Insights and Implications for Host Metabolic Health](#)
- [Metabolomics Facilitate the Personalized Management in Inflammatory Bowel Disease](#)
- [Metabolomics for Personalized Medicine: The Input of Analytical Chemistry from Biomarker Discovery to Point-of-care Tests](#)
- [Metabolomics in the Understanding and Management of Hepatic Encephalopathy](#)
- [Multiomics Approach Reveals a Role of Translational Machinery in Shaping Maize Kernel Amino Acid Composition](#)
- [Multiomics Integration-based Molecular Characterizations of COVID-19](#)
- [Multiomics Profiling of the Expression and Prognosis of MCMs in Endometrial Carcinoma](#)
- [Multiomics Subtyping for Clinically Prognostic Cancer Subtypes and Personalized Therapy: A Systematic Review and Meta-analysis](#)
- [Non-esterified Fatty Acids as Biomarkers of Diet and Glucose Homeostasis in Pregnancy: The Impact of Fatty Acid Reporting Methods: NEFA Reporting Methods Affect Dietary and Cardiometabolic Endpoints](#)
- [NP-MRD: the Natural Products Magnetic Resonance Database](#)
- [The Promise of Graphene-based Transistors for Democratizing Multiomics Studies](#)
- [A Roadmap to High-resolution Standard Microcoil MAS NMR Spectroscopy for Metabolomics](#)
- [Sex Differences in Alzheimer’s Disease: Insights From the Multiomics Landscape](#)
- [Subcellular metabolomics: Isolation, measurement, and applications](#)
- [Training Associated Alterations in Equine Respiratory Immunity Using a Multiomics Comparative Approach](#)
- [Untargeted GC-MS Metabolomics Reveals the Metabolic Responses in the Gills of Chinese Mitten Crab \(\*Eriocheir sinensis\*\) Subjected to Air-exposure Stress](#)
- [Untargeted Metabolomics Analysis of the Serum Metabolic Signature of Childhood Obesity](#)



# Metabolomics Events

13 January - 1 December 2022

Bits & Bites 2022

Register [here](#).

## Overview

These courses hosted by the UC Davis West Coast Metabolomics Center are great for grad students, postdocs, and other STEM professionals.

Bits & Bites is an online course series that features in-depth topics in untargeted metabolomics. Each short course can be taken individually, or you can select multiple Bites. You will gain a deeper insight into current software, methods, and pitfalls. We've added multiple fundamental courses for those interested in learning the advantages and disadvantages of such topics as Mass Spectrometry, Lipidomics, Metabolism, and Gas Chromatography-MS in Metabolomics.

For more information check out our flyer or visit our website: <https://metabolomics.ucdavis.edu/courses-and-seminars/courses/217-bits-and-bites-2021>



**LEARN ONLINE** UC DAVIS WCMC PRESENTS: **BITS & BITES 2022** REGISTER TODAY

<b>1</b> Fundamentals of Mass Spectrometry   Jan. 13, 2022	<b>6</b> Introduction to Bayesian statistics in Metabolomics   May 5, 2022
<b>2</b> Fundamentals of Lipidomics   Feb 3, 2022	<b>7</b> Identification of unknown compounds in untargeted metabolomics using freely available software Session I & Session II   Sept. 8-9, 2022
<b>3</b> Using MS/DIAL to generate accurate comprehensive LC-MS/MS metabolomics datasets   Mar. 3, 2022	<b>8</b> Introduction to Metaboanalyst   Oct. 6, 2022
<b>4</b> Introduction to the GNPS Ecosystem - Tools, Visualizations, and Data   Mar. 31, 2022	<b>9</b> Fundamentals of Gas Chromatography-MS in Metabolomics   Nov. 3, 2022
<b>5</b> Fundamentals of Metabolism   Apr. 7, 2022	<b>10</b> How to navigate demands in Metabolomics core services   Dec. 1, 2022

Registration fee: \$150 per bite. Sign-up for all 10 bites by Jan 10, 2022 to get an EARLY BIRD SPECIAL!

## 18 January 2022

### Startup TNT Life Sciences Investment Summit Application Deadline

Learn more [here](#).

#### Overview

The Startup TNT Life Sciences Investment Summit, a platform for life sciences entrepreneurs and innovators seeking seed stage funding and will provide them with an opportunity to receive seed funding for their idea or business, and to network with investors and representatives from the start-up and the life sciences ecosystem. The summit also offers hands-on training for investors interested in Life Sciences through a team-based due diligence process.

Applicants shortlisted by the investors will be invited to participate in an 8-week due diligence process. You'll have an opportunity to build relationships and engage with investors and mentors as a direct outcome of your participation in this process.

## 24-28 January 2022

### Hands-on LC-MS Data processing and Statistics

Learn more [here](#).

#### Overview

This course offered by UC Davis will feature hands-on training with real-world untargeted metabolomics data covering LC-MS data processing, compound identification, statistical analysis, network mapping, & data interpretation.

- Untargeted data processing and exercises on MS-DIAL software.
- Exercises on the identification of unknowns by cheminformatics software workflows (including MS-FINDER, CFM-ID, various databases, and small software routines)
- Data normalization and transformation with and without internal standards and quality controls
- Multivariate and univariate statistics
- Pathway mapping and enrichment analysis

## 15 February 2022

### Work-integrated Learning Industry Voucher (WILIV) Program

Learn more [here](#).

#### Overview

BioAlberta will use WILIV to support a total of 136 unique (16-week long) full time life science and STEM student internships to qualifying Alberta small and medium sized enterprises (SMEs) who successfully recruit skilled students enrolled in an under-graduate, graduate or post-graduate degree programs.

SME internships must provide students with practical work in a field related to their studies within the Alberta life sciences eco-system that enable them to gain a better understanding of your company's work. Eligible SMEs will be awarded \$5000 in matching wage support per student placement.



These Alberta SMEs are then free to match WILIV support with either their own operational funds or apply to other available student funding programs (i.e. BioTalent Canada, Eco Canada, etc).

BioAlberta is now recruiting SMEs to participate in WILIV Summer and Fall 2022. For more information or to apply contact [trish@bioalberta.com](mailto:trish@bioalberta.com).

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## 22-25 February 2022

### 6<sup>th</sup> HBP Student Conference on Interdisciplinary Brain Research

Learn more [here](#).

#### Overview

The 4-day conference will be held in a hybrid format with most sessions being streamed online. Participation in the 6<sup>th</sup> HBP Student Conference is open to the entire student community and early career researchers, regardless of whether they are affiliated with the HBP or not. Participants without contributions to the scientific programme are also welcome. We encourage all young scientists to register and aim for an equal representation of all genders.

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## 7-8 April 2022

### Course Data Analysis for Metabolomics

Register [here](#).

#### Overview

Metabolomics experiments based on mass spectrometry (MS) or nuclear magnetic resonance (NMR) produce large and complex data sets. This course will introduce approaches to process and analyze data and design high-quality experiments. Through hands-on workshops and lectures highlighting the different concepts you will get a thorough basis for tackling the challenges in metabolomics data analysis.

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## 13-16 May 2022

### 2<sup>nd</sup> Metabolism in Health and Disease Conference

Learn more [here](#).

#### Overview

Topics will span diverse areas such as cancer metabolism, organismal metabolism in disease, metabolic pathway engagement in cell function, metabolites as signaling molecules, mitochondrial biology, nutrient sensing, metabolism in tissue homeostasis and repair, neurometabolism, and metabolism in host-microbe interactions.

Early-bird registration deadline is January 31, 2022

## 29 May - 2 June 2022

### International GCxGC Symposium

Learn more [here](#).

#### Overview

Monday to Thursday - Technical Program:

- 2022 John B. Phillips and Scientific Achievement Award Lectures
- 3.5 full days of live talks, posters and discussion sessions
- Opportunities to contribute virtual talks and posters
- In-person content will be available to virtual attendees
- Breakfasts, lunches and snacks included in registration

This is a hybrid event so as many delegates can attend as possible. If you register to attend virtually before January 25, you will be able to upgrade to in-person (if we hold an in-person meeting) at the early bird rate up until March 15th. [So grab your spot now!](#)

## 19-23 June 2022

### 18<sup>th</sup> Annual Conference of the Metabolomics Society

Learn more [here](#).

#### Overview

The meeting will be co-organized with the Spanish Society for Metabolomics (SESMET) and the Spanish Network for Metabolomics. Building on the success of previous years, the conference will present the latest advances in the field covering the major scientific themes of technological advances, bioinformatics, metabolomics applications in health and disease, exposomics and a focus on metabolomics in agriculture, plants, food and nutritional sciences. The scientific program will include plenary and keynote talks, parallel scientific sessions, poster sessions, sponsored luncheons and other networking events.

## 20-24 June & 20-23 September 2022

### CliMetabolomics

Learn more [here](#).

#### Overview

CliMetabolomics is a Franco-german Research Workshop that aims to better understand the plasticity of plants and to develop sustainable plants adapted to climate change.

CliMetabolomics offers training in analytical tools and an innovation management method to early career scientists.

The workshop lasts two weeks and consists of seminars, discussions and many practical courses.

## 7-12 August 2022

Gordon Research Conference on Lipidomics

## 22 August - 2 September 2022

International Summer Sessions in Metabolomics

## 26-27 October 2022

2nd International Diabetes and Metabolic Surgery Summit

# Metabolomics Jobs

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

## Jobs Offered

Job Title	Employer	Location	Posted	Closes	Source
Postdoctoral Position	Paris-Saclay Food and Bioproduct Engineering Research Unit	Agro Paris Tech, Paris, France	24-Jan-22	Various	<a href="#">MetaboNews Jobs</a>
Various Positions	Various	Various	1-Jan-22	Various	<a href="#">Metabolomics Association of North America Job Board</a>
Sr. Marine Education Specialist - Science Technology Centre (STC)	Woods Hole Oceanographic Institution	Massachusetts, USA	4-Oct-21	Until Filled	<a href="#">Careers@WHOI</a>
Postdoctoral Position	Fernandez Lab, School of Chemistry and Biochemistry, Georgia Institute of Technology	Georgia, USA	Sep-21	Until Filled	<a href="#">MetaboNews Jobs</a>
PhD Student and Post-doctoral Fellow Positions in Mass Spectrometry Metabolomics and Proteomics	Technion - Israel Institute of Technology	Haifa, Israel	29-Mar-21	Until Filled	<a href="#">MetaboNews Jobs</a>
PhD Research Project Opportunities, Centre for Integrative Metabolomics and Computational Biology	Edith Cowan University	Joondalup, Australia	16-Mar-21	Until Filled	<a href="#">MetaboNews Jobs</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 your 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.

- [Dr. Rustem Shaykhtudinov](#) - Seeking a Research or Lab Manager position to apply his extensive experience and knowledge in the area of NMR metabolomics and his skills in NMR instrumentation maintenance.
- [Dr. Paulina Samczuk](#) - Seeking an interesting Postdoc offer or other position which would allow her to develop herself.



# Want to see your content in MetaboNews?

Do you have an interesting story you would like to share with the metabolomics community? [Fill out this form](#) to learn more about contributing a Spotlight Article to MetaboNews.

Would you like to share your metabolomics story? [Fill out this form](#) to be featured as one of our MetabolInterviews.

Do you have a new publication that the metabolomics community should hear about? [Fill out this form](#) to have your publication featured in MetaboNews.

Are you searching for a highly qualified individual for your organization? [Fill out this form](#) to post your job in MetaboNews.



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Full page ad - \$450 CAD

Featured Job Posting - \$50CAD

Featured Event Posting - \$100CAD

Commercial Spotlight Article or Interview - \$300CAD

\*Prices do not include GST

Have any questions?  
Contact your MetaboNews team at [metabolomics.innovation@gmail.com](mailto:metabolomics.innovation@gmail.com)