# MetaboNews



Metabolomics Society News Spotlight Article Reporting Standards (mQACC) Recent Publications Conferences & Events Jobs Offered Wanted

The MetaboNews Team

The Metabolomics Innovation Centre metabolomics.innovation@gmail.com http://www.metabonews.ca/archive.html



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

## Metabolomics Society News Conference Corner

#### Metabolomics 2022 - Conference Summary

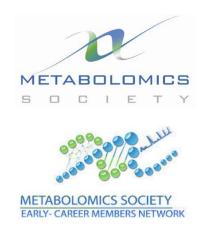
What a blast our conference in Valencia was! It was absolutely amazing to reunite as a scientific community in person after hosting two virtual conferences. We were delighted to see old friends reconnecting, witness new friendships being formed and sharing science on so many levels. Thank you to each and every one of you for making the conference such a memorable experience.

During the planning of the conference, we were concerned by the potential impact COVID-19 would have on registrations for our in-person meeting. We were thrilled to see an overwhelming response from the community with a total of 897 registrants from across the globe.



We were very pleased to receive 681 abstracts from which we constructed a diverse conference agenda, centred around four thematic streams comprising 4 plenary talks, 7 invited keynote presentations, 5 session keynotes (selected from abstracts), 103 oral presentations, over 500 posters, 8 sponsored talks during our dedicated vendors' session, and 4 sponsored lunch presentations. We are especially proud that we managed to put together a highly balanced line-up of speakers in terms of scientific topics, gender, geographical representation, and a very strong presence by early-career researchers.

#### October 2022 Metabolomics Society News



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

General Enquiries info@metabolomicssociety.org

Membership Enquiries membership@metabolomicssociety.org

#### Workshops

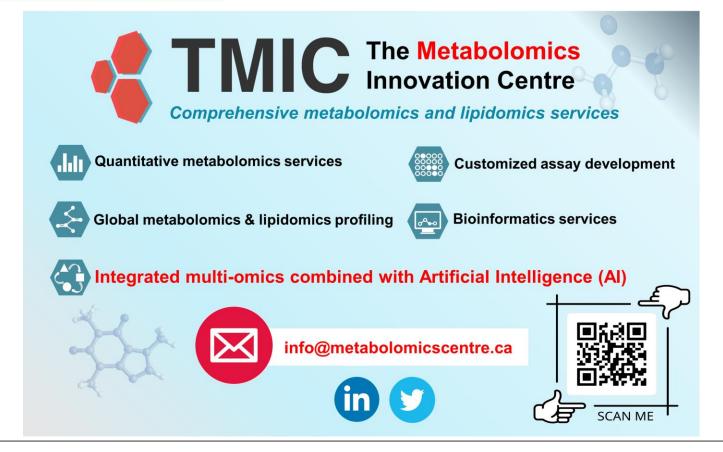
We kicked off the conference with 13 workshops covering all aspects of the field, from technology advancements, to data analysis, metabolite identification, metabolic epidemiology, and career development. We were thrilled to see such a great turnout and to receive excellent feedback on the quality of the workshops from attendees.

#### **Plenaries**

On day two we moved to the scientific sessions, kicked off by **Ron Heeren** (Maastricht University, Netherlands) who gave us a fascinating talk on molecular imaging in metabolomics. The third day started with a plenary talk by **Nicola Zamboni** (ETH Zurich, Switzerland) on the highly relevant topic of the democratization of untargeted metabolomics for its wider integration in discovery and clinical workflows. **Asaph Aharoni** (Weizmann Institute of Science, Israel) was our third spectacular plenary speaker who presented his group's work on ultra-resolution plant metabolomics and their pioneering work on metabolite identification and spatial metabolomics. Our plenary sessions concluded with **Coral Barbas** (Universidad San Pablo CEU, Spain) who gave us a truly enlightening talk on the most significant analytical challenges in the field of metabolomics.

#### 2022 Honorary Fellows of the Metabolomics Society

An Honorary Fellowship is a significant lifetime award granted by the Board of Directors of the Metabolomics Society to recognize exceptional members of the community who have either made outstanding.



contributions to the Metabolomics Society over a sustained period of time, and/or made a pioneering and sustained contribution to the science of metabolomics at an international level. With up to two lifetime Fellowships awarded each year, the Board is pleased to recognize the following individuals as the lifetime Honorary Fellows of the Metabolomics Society for 2022:

**David Broadhurst, PhD.** David has had a tremendous impact on the field of metabolomics through establishing and promoting practices for statistical rigour, experimental design, quality control, and clinical metabolomics methodology. His contributions to the Society are many and include serving on the Board of Directors as well as participation in multiple task groups, workshops, publications, and lectures.

Lorraine Brennan, PhD. Lorraine has had a tremendous impact on establishing the field of nutritional metabolomics, through the identification of dietary biomarkers and the implementation of dietary interventions, moving the field toward personalized nutrition. Her contributions and leadership within the Metabolomics Society is also truly exemplary and include chairing the annual Society conference in Dublin, Ireland, in 2016 and participation in multiple workshops, task groups, lectures, and publications.

#### **2022 Career Medal Recipients**

The Metabolomics Society seeks to recognize outstanding contributions to the field of metabolomics through the presentation of the Metabolomics Society Medals. They are open to all Society members who meet the eligibility criteria outlined below. While research contributions are of primary importance, other contributions, including the teaching of metabolomics and/or service to the field or the Society will also be strongly considered. There are up to two medals awarded each year in the following categories:

• 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 closing date for nominations in each round.

• The **President's Award** recognizes outstanding achievements in metabolomics by younger members of the Society. It is available for Society members who have been awarded a PhD no more than 5-10 years prior to the closing date for nominations in each round.

The Board of Directors is pleased to recognize the following individuals as the award recipients for 2022:

#### The Metabolomics Society Medal

María Eugenia Monge, PhD, Centro de Investigaciones en Bionanociencias (CIBION)

#### The President's Award

**Rachel Kelly, PhD,** Brigham and Women's Hospital and Harvard Medical School

We congratulate both award recipients and look forward to their continued contributions in the years to come.

#### **Other Awardees**

#### Metabolomics Society Travel Awards, Students:

Elys Rodriguez, Kieran Tarazona Carrillo, Maria Llambrich, Matthew Smith, Maxime Delmas, Niek De Jonge, Qishun Zhou, Tessa Peters, Yingxiao Yan, Zach Rabow

#### Metabolomics Society Travel Awards, Early Career Researchers:

Abhishek Jain, Alice Flint, Ilias Thomas, Jin Xu, Julia Debik, Kapil Dev Singh, Marta Moreno-Torres, Miguel Fernández-Niño, Nicole Prince, Susana Alejandra Palma Duran

#### **Evening Events**

#### **Career Night**

On Sunday evening, we hosted the second edition of our Career Night which was organized by the Early-Career Members Network (EMN) Committee. This dynamic event featured representatives from several employment sectors who had the opportunity to engage with job seekers. The event also included interactive round table discussions across a diverse range of topics



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pertaining to career and personal development. This event also included booths for job opportunities and one-on-one mentoring.

#### **Town Hall Meeting**

Our annual Town Hall meeting took place on Monday evening during which the membership had the chance to engage with the Board of Directors of the Society and hear about the current standing of the Society. We would like to thank those who attended and for the very constructive feedback, we received that will help guide the future plans of the Society.

#### **EMN Reception**

The EMN Committee is truly vital to the Society and this year they exceeded all expectations with the conference activities they organized. The EMN reception was no exception to this. During the event, the EMN Committee Chair, Evelina Charidemou, gave an overview of the EMN and its activities and presented the EMN travel bursary recipients with their awards. **Congratulations to Chanel Pretorius, Diana Pinto, Giorgia La Barbera, and Abhishek Jain.** The EMN also honoured Krista Zanetti for her invaluable contributions to the Committee. The evening concluded with a thoroughly entertaining and lively quiz!

#### **Conference Dinner**

A truly memorable evening! The conference dinner took place in Veles e Vents, one of Valencia's most iconic buildings with breath-taking views of the city. We enjoyed delicious Spanish food, had drinks watching the sunset, and danced the night away.

#### **Conference Sponsors**

We would also like to express our gratitude to our generous sponsors whose contributions made the event possible:

- Platinum: Agilent, Bruker, SCIEX, ThermoFisher Scientific
- Gold: Biocrates, LECO, Metware, Shimadzu
- Silver: BASF Metabolome Solutions, BGI Europe, Fossiliontech, IROA Technologies, Metabolites (MDPI), Cells (MDPI), MERCK, MetaKey, oloBion, Waters
- University/Non-Profit: TMIC

#### Thank you!

Thank you to the members of the Scientific Organizing Committee for their invaluable contributions towards



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shaping the scientific content of the conference. Thank you to the Conference Committee and Board of Directors of the Metabolomics Society for their constant input on all conference aspects. Lastly, we would like to thank SnapIT Solutions, our professional conference organizers, whose help and guidance was central to the success of the conference.

#### **Conference photos:**

https://www.metabolomics2022.org/conferencephotos

Conference videos and poster gallery (available to view on the OnAIR platform until October 31, 2022): https://portalapp.metabolomics.eventsair.com/Virtual AttendeePortal/metabolomics-2022/22met/login

#### Save the date for Metabolomics 2023!

With the 2022 conference behind us, we are now well underway with our preparations for next year's conference. The 19th edition of the Metabolomics Society conference will be held from June 18-22 at Niagara Falls, Canada. Follow all updates on https://www.metabolomics2023.org/

### International Affiliates' Corner

#### <u>Metabolomics Association of North America</u> (MANA)

Visit https://metabolomicsna.org

The 4<sup>th</sup> Annual MANA Conference was held September 16-18, 2022, on the campus of the University of Alberta in Edmonton, Alberta, Canada, and was a great

success! It was so nice to see our colleagues again in "three dimensions" for the first time in three years. Just the second in-person MANA conference, 250 earlycareer members, established investigators, and corporate members attended a program featuring instructional workshops; interactive forums; plenary, contributed and lightning talks; corporate member breakfast and lunch seminars; poster sessions; and award lectures. Many thanks to Professor David Wishart and the Local Organizing Committee! Importantly, 67% of attendees were early-career members, and 60% of registrants were participating in their first MANA conference, highlighting the future leaders in metabolomics and the still-growing nature of the Association. MANA prides itself on its ability to support its members and Early Career Members (ECM) by providing several different awards and grants. This year, we awarded 37 different awards and grants. Congratulations to all the MANA 2022 awardees!

#### MANA Early Career Rising Star Award

• Tao Huan | Assistant Professor, University of British Columbia

Awarded for his work in the development of analytical and bioinformatics tools for improving data acquisition and analysis of LC-MS-based metabolomics.

#### Mark P. Styczynski Early Career Award in Computational Metabolomics

• Sadjad Fakouri-Baygi | Postdoctoral Fellow, Icahn School of Medicine at Mount Sinai

Awarded for his work in the design, development, and support of new algorithms for processing untargeted high-resolution mass spectrometry data in the metabolomics and exposomics field.



PATHWAYS"

AWARDEES

ASSAY FOR TARGETED ANALYSIS OF MULTIPLE

LAUREN BISHOP | UC DAVIS | "TISSUE-SPECIFIC, ADDUCT

IAN HAN | UNI. OF CALGARY | "SERUM METABOLITE PREDICTORS

ECM LIGHTNING TALK

FORMATION AND LIPID QUANTIFICATION"

**OF PRETERM BIRTH IN PRIMIGRAVIDA"** 

Graduate Students KYLE SPENCER | NATL CNTR ADV TRANS SC KHYATI MEHTA | CINCINNATI CHILDREN'S HOSPITAL MICHAL LAZAREK | UNI. OF ALBERTA THOMAS HEAD | UBC YONGSEOK KIM | OHIO STATE UNI.

Undergraduate Students EWENET MESFIN | UNI. OF ALBERTA ABBY KROPIELNICKI | UNI. OF ALBERTA

**#MANA2022** 

**Emerging Leader Award in Metabolomics Service Cores** 

 Armando A. Magaña | Metabolomics Project Manager, Life Sciences Institute, University of British Columbia

Awarded for his work in advancing metabolomics science through leadership in service cores, specifically in the design and initiation of a new core and with the continued support of trainees and collaborators.

#### WomiX Mentorship Award

• Susan Murch | Professor, University of British Columbia



Polish Metabolomics Society Visit <u>https://ptmet.pl/</u>

The Polish Metabolomics Society (Polskie Towarzystwo Metabolomiczne) is inviting participants to the 9th Metabolomics Circle meeting. The conference will take place in Wrocław on January 27-28, 2023, and will be organized by Professor Piotr Młynarz from the Wrocław University of Science and Technology. Information about abstract submission and registration will soon be posted on the webpage.



of strong mentorship and leadership skills.

ECM Travel Awards were awarded to 15 ECM recipients!

Awarded for her demonstration

ECM Childcare Grants were awarded to 2 ECM recipients!

## SpOtlight

Reporting Standards for Quality Control Samples in Untargeted Metabolic Phenotyping

Jennifer Kirwan and Ian Wilson

Co-Chairs reporting on behalf of the Reporting Standards Working Group of the Metabolomics Quality Assurance & Quality Control Consortium (mQACC)

The debate about reproducibility in science, or the apparent lack of it, is again under discussion as, even where there is no suggestion of deliberate fraud, studies have often proved to be difficult to replicate [1]. Given that this is seen to be a problem for all areas of science it would be remarkable indeed if these difficulties did not also extend into our own field, especially untargeted metabolite profiling (metabolomics, metabonomics, metabolic phenotyping). And, given the myriad differences between laboratories, analytical techniques, instruments, procedures, and sample types, it should not come as any sort of surprise that there can be vigorous debates about the results of untargeted metabolomic analyses. Now, showing that different methods produce different results need not be a problem as this can often result simply from the different selectivities of those methods. For example, it would surprise no one if urine samples analyzed by <sup>1</sup>H NMR spectroscopy and reversedphase liquid chromatography (LC) identified some different compounds as potential biomarkers. Indeed, such differences are accepted as the natural course of things, and both sets of data are accepted

Quality Assurance & Quality Control Consortium (mQACC)

Promoting the development, dissemination and harmonization of best QA/QC practices in untargeted metabolomics

as being valid. In addition, the platform-specific validity and quality of the data obtained, by both platforms, can also be easily demonstrated by reporting the results obtained for the quality controls (QCs) for both methods. However, where a problem would arise would be if, for example, in the case of the <sup>1</sup>H NMR spectroscopic data, hippuric acid was seen to be present in relatively higher concentrations in the test group compared to the controls, but in relatively lower concentrations by LC/MS. Such contradictory results should result in a very rapid reappraisal of the quality of the data as both sets of observations could not possibly be correct. In such cases, the value of properly-applied QC procedures would be of great help to pinpoint the nature of the problem by highlighting or eliminating poor analytical results, for one or other of the methods used, and suggesting that some other factor was at work (e.g., matrix effects on ionization, interfering peaks, etc.). In addition, as to the difference due to the mode of analysis, it has long been known that for LC/MS, even when the same LC separation is used, both the MS used to detect the metabolites and the software employed to analyze

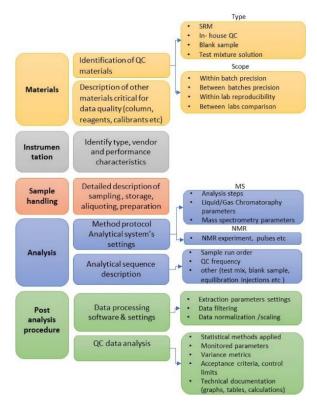
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the data can affect the results [2] and this has obvious implications for multi-laboratory studies where instrumentation differs between sites. However, the use of properly-acquired, properlyinterpreted, and well-*reported* QC data can help to solve many of the challenges associated with accepting the results obtained in untargeted "discovery" metabolic phenotyping studies, and this, at least in part by it being able to demonstrate unequivocally that the data have been produced in a metabolomics study environment that is of sufficiently high quality to be trusted and appropriately interpreted. Gaining and maintaining this trust is essential in ensuring the acceptance of our work, by our colleagues, our customers (biochemists, clinicians, epidemiologists, etc.), and our other stakeholders (patients, the public, grantawarding bodies, etc.). The use of quality assurance (QA) and quality control (QC) protocols is widely accepted as best practice in analytical chemistry and provides a firm foundation on which to build such trust. The Metabolomics Quality Assurance and Quality Control Consortium (mQACC) was formed in 2017, following in the footsteps of the Metabolomics Society's Data Quality Task Group [3,4] with the aim of engaging with the metabolomics community to communicate and promote the development, dissemination, and harmonization of best QA/QC practices in untargeted metabolomics.

Specifically, the aims of the mQACC are

- to identify, catalogue, harmonize, and disseminate QA/QC best practices for untargeted metabolomics;
- to establish mechanisms to enable the metabolomics community to adopt QA/QC best practices;
- to promote and support systematic training in QA/QC best practices for the metabolomics community; and
- to encourage the prioritization and development of reference materials applicable to metabolomics research.

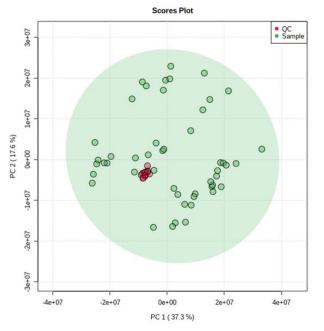
And mQACC has proceeded to do this with workshops, surveys, and publications ever since. Much of this work has been undertaken by subsets of the membership of mQACC in working groups looking at various topics (e.g., see refs 5-9). One of the topics recently covered by these working groups has been "Reporting Practices" for publications containing untargeted metabolomics data [9]. This has initially concentrated on how best to report the QC aspects of untargeted metabolomic analysis in such a way as to instill confidence in the reader that the reported study sample analysis had been well performed and to better understand the technical limitations of the dataset, thus enabling more confident interpretation of the biological results. Most metabolomics groups these days utilize protocols, including system suitability tests (SSTs) and QC samples of one sort or another, to monitor the analytical system prior to and during the analytical process (see Figure 1). Indeed, such



**Figure 1.** Information that should be documented in manuscripts to show the steps that have been taken to ensure the robustness of the analytical stages of a metabolic phenotyping experiment and its resulting data. Taken from ref 9 with permission of the copyright owners.

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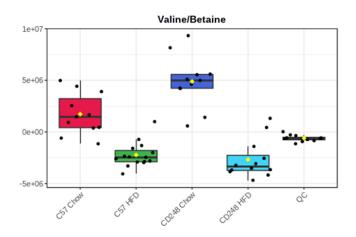
practices remain an important part of the untargeted metabolomic analysis and one that continues to evolve. However, the often-inadequate reporting of the QA/QC procedures used in studies is, in our experience, a common feature of many papers. Therefore, encouraging authors to proactively show that the analytical work underpinning their investigations had been well performed was seen as a priority that would allay many doubts about the reliability of metabolomics research. Our aim as highlighted in the recently published mQACC guidance [9] was therefore to provide authors with encouragement and advice on providing detailed descriptions of the QA/QC systems employed in their analytical work and the outcomes of their efforts in this area. Whilst concentrating on MS- and NMR spectroscopy-based analysis, the guidance can easily be adapted to other methods used in untargeted metabolomics. In particular, these suggestions focus on the detailed reporting on the use of QC samples



**Figure 2.** A fairly typical principal component analysis (PCA) for the LC/MS of mouse urine samples (green data points) showing the QC samples (red data points), prepared by making pooled urine samples from aliquots of all the test samples, forming a tight cluster in the score plot, providing initial evidence to suggest the absence of major run order effects, etc., and some confidence that further detailed analysis of the data obtained for both QC samples and test samples can be justified. Adapted from ref 10 with permission of the copyright owners.

(see **Figures 2** and **3** for examples) so that another analytical chemist, skilled in the art of untargeted metabolic phenotyping, could understand what was done, to replicate it if need be, and trust the results presented in the manuscript. We emphasize that the paper is deliberately not prescriptive and does not try to define best analytical practices in this area.

Instead, we want to encourage authors to accurately *report* their QA/QC procedures and results. To assist in this task, the paper proposes a list of standard quality management measures (QA and QC) that are undertaken at most labs undertaking untargeted metabolomics studies to assess and evaluate the analytical quality of data. Reporting of the procedures and results of these quality measurements have been further divided into minimal and best reporting practice standards. Such reports centre around the use of QC samples but also cover other aspects of QA such as system suitability tests. Topics considered for inclusion in reports include the sources, types, and preparation of the QC materials themselves and their use. In addition, the provision of descriptions of the use of test mixtures, system suitability tests, blanks, and sample



**Figure 3.** Following the identification of a potential biomarker from the untargeted LC/MS data obtained from test and control groups of mice, the variability of the analytical data for that analyte can be quickly examined by comparing the biological variability against that of the pooled QC samples (far right in the box plot). In the example shown here, the biological variability is clearly much higher than that of the analytical methodology. Adapted from ref 10 with permission of the copyright owners.

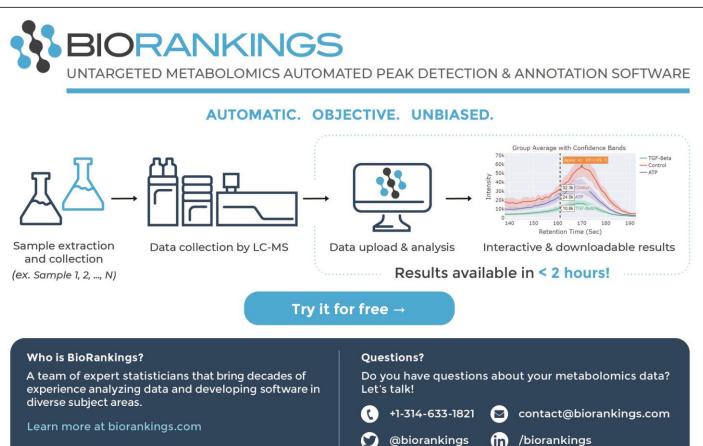
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preparation, etc., are recommended. Further and importantly, the reporting of the acceptance criteria used for the QCs is also discussed.

We believe that since much of the data required for reporting these factors is already being routinely collected, employing these "best reporting practices" should require little extra work. To reduce the workload further, we have developed examples of templates that can be populated with the required data as it becomes available. These templates can then be submitted as supplementary information on publications to complement the most important aspects of the QC work reported in the main manuscript (see the **Online Resources** provided with ref 9).

We are of course aware that many groups have welldeveloped QA/QC protocols but, as yet, no real consensus exists on how to report these in publications. Given the importance to the metabolomics community of being able to gauge their effectiveness in ensuring the quality of the resulting data, we believe that these guidelines represent one step towards defining the best reporting standards and engaging both researchers and publishers in this debate. It is our hope that, in this way, we can promote a vigorous debate within the metabolomics community and work towards achieving a broad consensus as to what constitutes the standard for the provision of these data. As such it is inevitable that these recommendations will change in line with evolving analytical practices with regard to QA/QC. To enable input and encourage buy-in from the metabolomics community, it is our intention to hold a number of virtual meetings over the next 12 months to allow interested parties to provide their views and debate the points raised around the best reporting practices in this area. Hopefully from this sort of initiative, consensus on reporting practices will be reached. The meeting dates and times will be published on the mQACC website: <a href="https://www.mqacc.org/">https://www.mqacc.org/</a>



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But the bottom line has to be, if you used QCs in your studies, DO PLEASE TELL EVERYONE, in sufficient detail, in your papers what they were, how you used them, and what they told you about your analysis!

#### About the authors

#### Jennifer Kirwan



Dr. Jennifer Kirwan started her career as a clinical veterinarian where she became increasingly interested in translational and evidence-based

medicine before undertaking a PhD in metabolomics. She now heads the Berlin Institute of Health's Metabolomics Platform at Charité University Hospital in Berlin, where she focuses on translational health-related metabolomics, especially on its quality management aspects. She is particularly interested in the gut-brain-heart health triad and how the microbiome influences health. She is a founding member of the German Society for Metabolomic Research (Deutsche Gesellschaft für Metabolomforschung (DGMet)), a Coordinating Committee member of the international Metabolomics Quality Assurance and Quality Control Consortium (mQACC), and an active member of the Precision Medicine and Pharmacometabolomics Task Group of the international Metabolomics Society.

#### Ian Wilson



Following a degree at the University of Manchester Science Institute of and Technology (UMIST), Ian Wilson undertook doctoral research at Keele University in the 1970s and followed this with а brief period of postdoctoral research at University College London. He then embarked on a 30+ year career in the pharmaceutical industry, eventually becoming a

Senior Principal Scientist in the Department of Drug Metabolism and Pharmacokinetics at the AstraZeneca research site at Alderley Park. He moved to Imperial College London in 2012 to a Chair in Drug Metabolism and Molecular Toxicology (where he is now a Visiting Professor, as well as holding a similar position at Liverpool University). He has been actively involved in metabolic phenotyping (metabonomics/metabolomics), using both <sup>1</sup>H NMR spectroscopy and LC/MS, since the 1980s, applying advanced high-throughput analytical techniques to the metabolic phenotyping of drugs and toxins in search of mechanistic insight for their effects. In 2021, he was made a lifetime Honorary Fellow of the Metabolomics Society, at least in part for "his work to improve standards and data quality via the introduction of pooled samples for use in quality control". Currently, he is one of two joint chairs of the mQACC working group on Reporting Standards.

#### **References**

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- 10. Armitage, E.G., *et al.* Metabolic consequences for mice lacking Endosialin: LC–MS/MS-based metabolic phenotyping of serum from C56Bl/6J Control and CD248 knock-out mice. *Metabolomics.* 2021, 17, art. 14.

## **Recent Publications**

#### Recently published papers in metabolomics

- <u>Anti-Inflammatory Diet Prevents Subclinical Colonic Inflammation and Alters Metabolomic Profile of</u> <u>Ulcerative Colitis Patients in Clinical Remission</u> (Open access)
- <u>Bioinformatics strategies for studying the molecular mechanisms of fungal extracellular vesicles with a focus</u> on infection and immune responses (Review)
- <u>Cancer as microenvironmental, systemic and environmental diseases: opportunity for transdisciplinary</u> <u>microbiomics science</u>
- <u>Cross-feeding niches among commensal leaf bacteria are shaped by the interaction of strain-level diversity</u> and resource availability (Open access)
- Diversification of heat shock transcription factors expanded thermal stress responses during early plant evolution (Open access)
- <u>Emerging nanosensor platforms and machine learning strategies toward rapid, point-of-need small-</u> <u>molecule metabolite detection and monitoring (Open access)</u>
- <u>Integrative omics approaches for biosynthetic pathway discovery in plants (Review, Open access)</u>
- <u>Mapping the human gut mycobiome in middle-aged and elderly adults: multiomics insights and implications</u> for host metabolic health (Open access)
- <u>Metabolic subtypes of patients with NAFLD exhibit distinctive cardiovascular risk profiles (Open access)</u>
- <u>Multi-omic brain and behavioral correlates of cell-free fetal DNA methylation in macaque maternal obesity</u> <u>models</u> (Open access)
- <u>Nuclear magnetic resonance spectroscopy in extra virgin olive oil authentication</u> (Review, Open access)
- <u>Nut consumption is associated with a shift of the NMR lipoprotein subfraction profile to a less atherogenic</u> pattern among older individuals at high CVD risk (Open access)
- <u>Simultaneous prediction of risk for multiple common diseases using metabolomics</u>
- <u>The Prostate Cancer Androgen Receptor Cistrome in African American Men Associates with Upregulation of</u> <u>Lipid Metabolism and Immune Response</u> (Open access)
- <u>Towards a mechanistic understanding of microalgae-bacteria interactions: integration of metabolomic</u> <u>analysis and computational models (Review)</u>

## **Metabolomics Events**

## October 20-21, 2022

7th Gateway Symposium Venue: Online Learn More Here (updated link)

#### **Overview**

The 7<sup>th</sup> Gateway Symposium at the University of Kentucky is entitled "NMR in Metabolism: New methods & applications". The general topic areas are

- applications in metabolomics,
- applications of stable isotope tracers, and
- new methods/developments.

The speakers have been confirmed. Find out more in the above link.

## October 25-27, 2022

2nd International Diabesity 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's 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 (Latin American Metabolic Profiling Society) 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. The deadline for registration and poster abstract submission is **October 18, 2022**.

## **November 3, 2022**

Bits & Bites #9: Fundamentals of Gas Chromatography-MS in Metabolomics 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.

This 9<sup>th</sup> course is taught by Dr. Oliver Fiehn and Dr. Uri Keshet, both of UC Davis, with MS-DIAL for Windows and BinVestigate as required software. While LC-MS is all the hype in today's portfolio of metabolomics assays, ranges of small molecules are difficult to impossible to screen in this manner. Volatile compounds in breath, urine, or plant analyses can best be analyzed by GC-MS. Additionally, swaths of primary metabolic intermediates ranging from glycolysis and pentose phosphates to TCA compounds, sugars, and small microbial metabolites are readily and cost-efficiently analyzed by GC-MS. In this short course, we discuss fundamentals of GC-MS, tips for best practice, aspects of instrumentation, and demonstrate data processing and use of databases. Participants will also learn the current challenges, trends, and developments of GC-MS-based metabolomics.

## November 21-25, 2022

Hands-on Data Analysis for Metabolic Profiling (Training Course) Venue: Online Learn More Here

#### **Overview**

This 5-day course (offered by Imperial College London) provides a comprehensive overview of data analysis for metabolic profiling studies focussing on data from NMR spectroscopy and liquid chromatography-mass spectrometry (LC-MS). It combines lectures and tutorial sessions using open-source software to ensure a thorough understanding of the theory and practical applications. Early-bird registration deadline is **October 21**.

## December 4-7, 2022

The Human Microbiome: Ecology and Evolution Venue: Banff, Alberta, Canada; Online (Hybrid) <u>Learn More Here</u>

#### **Overview**

This Keystone Symposia conference will explore the evolutionary and ecological forces shaping the interplay between the human host and microbiome., and is held jointly with the conference "Novel Approaches Against Emerging Antimicrobial Resistance". The microbiome is implicated in a widening set of disease conditions, yet many questions remain as to how its diversity and composition are assembled and maintained. The abstract submission deadline is **October 23**.

## December 13, 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), 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.



-----2023------

## January 27-28, 2023

IX Metabolomics Circle Meeting Venue: Wrocław, Lower Silesian, Poland Learn More Here

#### **Overview**

The Polish Metabolomics Society (Polskie Towarzystwo Metabolomiczne) is inviting participants to the 9th Metabolomics Circle Meeting, which will be organized by Professor Piotr Młynarz from the Wrocław University of Science and Technology. Information about abstract submission and registration will soon be posted on the webpage.

## March 12-17, 2023

Gordon Research Conference: Metabolomics and Human Health Venue: Barga, Lucca, Italy <u>Learn More Here</u>

#### **Overview**

The Metabolomics and Human Health Gordon Research Conference (March 2023) will highlight state-of-the-art metabolomics technologies and how such technologies can be used to study human health. Applications for this meeting must be submitted by **February 12**, **2023**. Please apply early, as it may become oversubscribed (full) before this deadline.

## March 28-31, 2023

EMBL-EBI course | Introduction to Metabolomics Analysis Venue: Hinxton, Cambridgeshire, United Kingdom Learn More Here

#### **Overview**

The European Bioinformatics Institute (EMBL-EBI) is organizing an on-site course at the EMBL-EBI Wellcome Genome Campus in Hinxton. This course will provide an introduction to metabolomics through lectures and hands-on sessions, using publicly available data, software, and tools. It is an open application with a selection for 26 seats. Please submit all required documents for the application process by **January 2, 2023**.



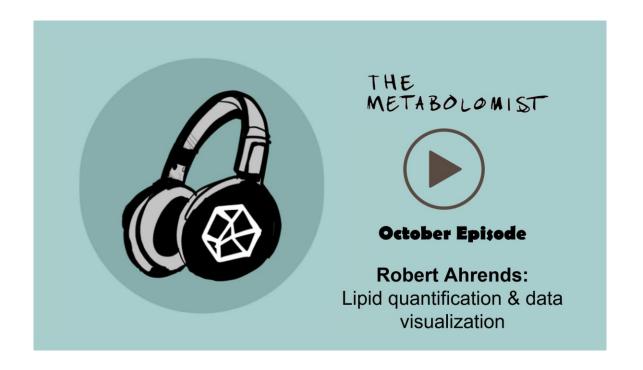
## June 18-22, 2023

19<sup>th</sup> Annual Conference of the Metabolomics Society Venue: Niagara Falls, Ontario, Canada <u>Learn More Here</u>

#### **Overview**

Save the date! Visit the website for updates over the coming weeks.

We are excited to put out an open call to the Society Members for workshop proposals. We are busy planning the conference agenda and eager for your input on pre-conference workshops. The workshops will provide a terrific venue to discuss a wide range of important topics and practical aspects of metabolomics, and may include hands-on learning opportunities. The deadline for the proposal submission is **November 10, 2022**.



## Metabolomics Jobs

## Jobs Offered

If you have a job to post, please email the MetaboNews team at <u>metabolomics.innovation@gmail.com</u>. 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	Posted	Closes	Source
Postdoctoral Research Associate (Metabolomics Core Technology Platform)	Heidelberg University	Heidelberg, Baden- Württemberg, Germany	19-Sep-2022	31-Oct-2022	<u>Heidelberg</u> <u>University</u>
Postdoctoral Fellows (Metabolomics, Proteomics, and Informatics - Microbial Infections)	University of Calgary	Calgary, Alberta, Canada	19-Sep-2022	Until filled	<u>Lewis Research</u> <u>Group</u>
Plant Metabolomics Research Fellow	US Department of Agriculture- Agricultural Research Service	Madison, Wisconsin, USA	14-Sept-2022	31-0ct-2022	<u>Oak Ridge</u> <u>Associated</u> <u>Universities</u>
Periodic Table of Food Initiative Research Scientist I	Colorado State University	Fort Collins, Colorado, USA	9- Sep-2022	Until filled	<u>Colorado State</u> <u>University</u>
Research Technician (Mass Spectrometry)	University of Alberta	Edmonton, Alberta, Canada	5-Sep-2022	Until filled	<u>University of</u> <u>Alberta</u>
Postdoc in Mass Spectrometry	University of Alberta	Edmonton, Alberta, Canada	1-Sep-2022	Until filled	<u>University of</u> <u>Alberta</u>
Operations Manager (TMIC-The Metabolomics Innovation Centre)	University of Alberta	Edmonton, Alberta, Canada	2-Aug-2022	Until filled	<u>University of</u> <u>Alberta</u>
Research Director – In vitro Diagnostics	Metabolomic Technologies Inc.	Edmonton, Alberta, Canada	20-Jun-2022	Until filled	<u>MetaboNews</u> <u>Jobs</u>
Postdoctoral Position in Metabolomics and Proteomics	Brigham and Women's Hospital	Boston, Massachusetts, USA	17-Jun-2022	Until filled	<u>Brigham and</u> <u>Women's</u> <u>Hospital</u>
Postdoctoral Research Fellow in Metabolomics (Diabetes)	Lund University	Lund, Sweden	15-Jun-2022	Until filled	<u>MetaboNews</u> <u>Jobs</u>

## Jobs Offered

Job Title	Employer	Location	Posted	Closes	Source
Post-Doctoral Researcher in Computational Metabolomics	Institute of Molecular Systems Biology, ETH Zurich	Zürich, Switzerland	14- Jun-2022	Until filled	ETH Zurich
Postdoctoral Research Fellow (Exometabolomics)	North Carolina State University	Raleigh, North Carolina, USA	13-May-2022	Until filled	<u>North Carolina</u> <u>State University</u>
Senior Associate Researcher in Mass Spectrometry	Icahn School of Medicine at Mount Sinai	New York City, New York, USA	6-May-2022	Until filled	<u>Icahn School of</u> <u>Medicine at</u> <u>Mount Sinai</u>
Postdoctoral Research Fellow (LC-MS and Data Science for Metabolomics)	University of Alberta	Edmonton, Alberta, Canada	4-May-2022	Until filled	<u>University of</u> <u>Alberta</u>
Assistant Professor in Metabolomics of Adaptive Responses	University of California, Riverside	Riverside, California, USA	15-Apr-2022	Until filled	<u>University of</u> <u>California,</u> <u>Riverside</u>
Various Positions	Various	Various (within North America)	Various	Various	<u>Metabolomics</u> <u>Association_of</u> <u>North America</u>

## 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 <u>metabolomics.innovation@gmail.com</u>. Upon review, a limited number of job submissions will be selected for publication in the Jobs Wanted section.