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## Metabolomics Society News

### Members Corner

#### Metabolomics Society 2020 – 2025 Strategic Plan for Membership Retention and Expansion

In 2017, the Society executed a broad survey of its members to assess the degree of its current success in achieving its mission, define opportunities for improving its service to the community, and make plans to establish the future goals and direction of the Society. The summary of our methodology and main findings of this evaluation have been published in *Metabolites* (2019, 9(5), 89; <https://doi.org/10.3390/metabo9050089>). In the publication, we also provide access to the results and make key conclusions defining how the Society should aim to move forward to continue to support community needs and promote metabolomics. The main findings of the survey were the basis for the development of the Society's Strategic Plan for Membership Retention and Expansion. A summary of the conclusions and strategic plan objectives are outlined below.

#### Main Conclusions from the Survey

Based on the survey results, areas for the Society to focus on to support member needs are:

- collecting and monitoring of demographic data during the membership registration process;
- continuing to support the early-career members of the Society through initiatives such as the EMN; and
- developing initiatives that focus on member networking to retain and increase Society membership, including increased interaction with the Society's local affiliates to identify specific needs for various geographical regions.

#### Strategic Plan Focus Area 1: Collect and Monitor Demographic Data During the Membership Registration Process

The Society collects minimal information at registration that includes no demographic information other than if the registrant qualifies as an early-career member, which is defined as being within five years of the attainment of a graduate degree. Therefore, the Society should consider collecting additional demographic data that are asked of all members upon registration, while still allowing any member to opt out of providing personal information if desired. Having sufficient member demographic data would position the Society better to determine what initiatives would best serve the membership and track trends over time. Furthermore, it would allow the Society to establish targeted recruitment efforts and determine if those efforts were meeting the established goals. Based on the survey, the Society should be targeting increased membership recruitment in Africa and South America; however, without collecting these data from member registrations, it won't be possible to evaluate whether recruitment effort initiatives are successful.

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

**Focus Area 1 Objectives:**

1. Revitalize the Society's Membership Committee to lead this focus area by January 31, 2020.
2. Determine what demographic data should be collected at the point of member registration by July 31, 2020.
3. Implement strategies for targeted membership recruitment in Africa and South America by September 30, 2020.  
The Membership Committee should work in conjunction with the South African Affiliate to identify specific needs for this region.
4. Establish a procedure for monitoring key data to determine if the Society is meeting its recruitment and retention goals by September 30, 2021.

**Strategic Plan Focus Area 2: Continue to Support the Early-Career Members of the Society**

The survey data showed that a significant portion of the Society membership was in training positions. Additionally, 80% of respondents had been in the field less than 10 years. Forty-seven percent of those respondents had been working in the field less than 5 years, which primarily reflects early-career members. This suggests the still nascent nature of metabolomics and the continued adoption of the technology by additional research groups. To support this sector of the membership, the Society established the Early-career Member Network (EMN) Committee in 2013 to provide a forum for metabolomics researchers at the start of their professional career and serve the early-career members of the Metabolomics Society. The EMN Committee has several ongoing projects and initiatives including a webinar series, bursary program for early-career members to travel to conferences, and organization of workshops and a reception at the Annual Meeting. Additionally, members of the EMN Committee participate on several Society Committees and Task Groups, and the Chair of the EMN Committee holds a position on the Society Board of Directors. Survey respondents considered one of the most important initiatives/activities currently supported by the Metabolomics Society to be the EMN.

Although the broad membership agreed that networking and the annual meeting were the most important benefits of being a Society member, trainees held career development opportunities as being more important than the senior, more established members of the Society. Specifically, those initiatives/activities that were more important to trainees were job postings on the website, opportunities to apply for travel awards, opportunities to apply for conference support, and membership in the Early-career Member Network. The Society provides travel awards to the annual meeting for early-career members. Additionally, in 2018, the EMN established a bursary program to support increased participation of early-career researchers at both the Society's annual meeting and other metabolomics-focused conferences. Considering the significant presence of early-career scientists within the membership, the Society should review the current career-development focused initiatives and consider expanding them to include additional support.

**Focus Area 2 Objectives:**

1. In collaboration with the EMN Committee, review survey data and ongoing career-development initiatives to identify gaps in support for this sector of the membership by July 31, 2020.
2. In collaboration with the EMN Committee, identify and subsequently establish/expand key initiatives/programs for continued support of early-career members by July 31, 2021.
3. Identify and implement novel opportunities for early-career members to network with their peers and senior Society members by July 31, 2022.

**Strategic Plan Focus Area 3: Develop Initiatives Focusing on Member Networking to Retain and Increase Society Membership**

The survey data showed that 72% of respondents had attended a Metabolomics Society Annual Meeting; however, only 38% remained a Society member in the years that they do not attend the annual meeting. This suggests that the Society should develop additional incentives to retain members even when they do not attend the annual meeting. Respondents felt that best strategies to maintain the current membership to be increased networking among members and increased opportunities to participate in annual meetings, which provides members an opportunity to network. Furthermore, respondents considered the best strategy to increase membership to be increased networking among members. This was consistent regardless of professional status; therefore, increased opportunities to network across the broad membership



**METABOLOMICS SOCIETY**  
EARLY-CAREER MEMBERS NETWORK

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)

Several activities have recently been held at the annual meeting to increase networking opportunities. The EMN holds a reception for early-career members to network with their peers and the Board of Directors. Additionally, regional affiliates have held receptions to encourage those in geographical proximity to each other to network and join their local affiliates. Based on the survey, these types of activities are in line with what the membership regards as the most important strategy to maintain and increase Society membership. However, additional networking opportunities should be explored and established for the full membership and in conjunction with the Society's regional affiliates.

#### Focus Area 3 Objectives:

1. Revitalize the Society's Membership Committee to lead this focus area by January 31, 2020. The Membership Committee should work in conjunction with the International Affiliations Task Group to identify specific needs for various geographical regions.
2. Evaluate current Society networking opportunities by September 30, 2021.
3. Identify and implement opportunities/initiatives/programs to increase networking across the broad membership to both maintain and retain members by September 30, 2022.

#### Evaluation of Strategic Plan

In addition to implementing the strategic plan, the Society should establish an evaluation plan to monitor progress toward achieving and completing the proposed objectives. This will allow the Society to demonstrate the impact of the strategic plan, as well as increase the productivity and effectiveness of the strategic plan throughout the duration of implementation. Evaluation will also provide data for the establishment of the 2025-2030 strategic plan. Equally important, an evaluation plan will provide data that can be shared with the membership to increase transparency.

#### Objectives:

1. Society Strategy Task Group will develop and implement an evaluation plan in collaboration with the Board of Directors, Membership Committee, International Affiliations Task Group, and Early-Career Member Network Committee.
  - a. Focus Area 1 by September 30, 2021.
  - b. Focus Area 2 by July 31, 2022.
  - c. Focus Area 3 by September 30, 2022.
  - d. Data collection and reports to the membership through September 30, 2025.

### Early-career Members Network (EMN)

#### Travel Bursary Program

We want to congratulate the outstanding winners of this year's Travel Bursary Program: Georgia Sinclair (RMIT University, Melbourne, Australia), Melanie Odenkirk (North Carolina State University, USA), Lili Herendi (Imperial College London, UK), Purva Kulkarni (Radboud University Medical Center, The Netherlands), Guy Schleyer (Weizmann Institute of Science, Israel).



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### EMN Webinars

We are delighted to announce that Drs. Justin van der Hooft and Madeleine Ernst will present their research at the next EMN webinar on June 19th, 2020. Registration links and announcements will be sent over email and posted on our social media platforms.

### EMN Social Media

Follow the EMN on [Facebook](#) and [Twitter](#) for updates and special events.

### Applications are open for Section Editor positions with *Metabolites*



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*Metabolites* (<https://www.mdpi.com/journal/metabolites>) is an international open access journal led by Editor-in-Chief Prof. Dr. Peter Meikle from the Baker Heart and Diabetes Institute, Australia. *Metabolites* is devoted to all areas of metabolism and metabolomics and is published monthly online by MDPI. It is indexed in SCIE, with a latest Impact Factor of 3.303. It ranks 126/298 (Q2) in "Biochemistry & Molecular Biology. *Metabolites* is the official journal of the Metabolomics Society (MetSoc).

To accommodate the increase in manuscript submissions and to better focus the activities of the journal we have introduced journal Sections (<https://www.mdpi.com/journal/metabolites/sections>). We also intend to expand the Editorial Board of the journal. Applicants for Section Editor should be mid to senior level researchers and may propose a specific section in which they feel their expertise lies.

Section Editor tasks entail:

- Scientific discussion or strategy about the journal's aims and scopes
- Invite distinguished scientists to join the Editorial Board
- Suggest topics for Special Issues or hot topics on your section
- Overview of the editorial process of the manuscripts on your section (mainly preview new submissions and make the final decision on whether a paper can be published after peer-review and revision).

The Section Editor position is honorary. We invite you to publish two papers per year free of charge. The term for the Editorial Board position is 2 years and can be renewed.

We believe that your expertise together with our rigorous editorial policies can help build a high-quality journal specifically dedicated to metabolism and metabolomics research. If you are interested in becoming a Section Editor for Metabolites, please send your full academic CV and a short cover letter that details your interest and enthusiasm for the position. Please also indicate the sections you feel match your expertise and interest. The documents should be sent to [metabolites@mdpi.com](mailto:metabolites@mdpi.com) before 30 June 2020.

We look forward to hearing from you.

## Special Issue Announcement from Metabolites

I hope you are all coping with the unprecedented changes that are occurring in the wake of COVID19. This is having a tremendous impact on the way we work and live. It appears that it will be some time before things start to normalise and indeed, I suspect things will never be the same after an event such as this. We can only hope that the signs of cooperation we have seen within and between governments might continue beyond the current pandemic.

With the majority of us likely working remotely, with limited access to our laboratories, I expect that many of you will be looking to complete analyses and manuscripts over the coming months. To this end I would like to draw your attention once again to our Special Issue “10th Anniversary of Metabolites: The Changing Landscape of Metabolomics” and consider a submission.

You can see details of this Special Issue at:

[https://www.mdpi.com/journal/metabolites/special\\_issues/10\\_anniver](https://www.mdpi.com/journal/metabolites/special_issues/10_anniver)

Wishing you all the best over what are sure to be challenging times.

-Peter

Professor Peter J Meikle, Editor-in-Chief, Metabolites

## Notes from the Chair

This month the Board is normally gearing up for the International meeting which this year would have taken place in the first week of July in Shanghai. Alas, it was not to be this year. Personally, it's been a particularly bleak month where we have lost colleagues and loved ones to COVID-19. I was particularly shocked by the death of Prof. Michael Wakelam who has been a champion of lipidomics (and metabolomics) in the UK for the last couple of decades (possibly more!) and I urge you if you have a moment to read about his legacy in his obituaries in Metabolomics, the Journal of Lipid Research and Nature Metabolism. His work has been a real education in how you characterise some of the most unforgiving lipid signalling molecules to understand fundamental cellular processes.

However, there are chinks of light shining through the dark clouds. Many of you will have seen (and possibly joined) the consortium of mass spectrometrists that have come together to tackle COVID-19 and wrote an open letter to the Lancet (The COVID-19 Mass Spectrometry Coalition if you are interested in joining). Recently Markus Ralser (for disclosure a former office mate) has published his ground breaking work in Cell using mass spectrometry to discriminate between mild and severe COVID-19 infection.

As part of the Board's spirit of optimism we have begun organising a virtual meeting of the Society this year. While we can't recreate all the excitement of the face to face meeting we would have had this year in Shanghai, we can virtually come together as a community to discuss science, build networks and showcase the very best of metabolomics research across the globe. The meeting will be held from the **27th-29th October** with day 1 consisting of workshops and days 2 and 3 of research sessions.

## Metabolomics Society News | *Notes from the Chair*

We have plans for a virtual poster competition to pick the best posters for flash and short presentations during the main conference sessions. As an international organisation, we wanted to make sure the first virtual meeting of the society was also international in nature. So, for those old enough to remember we have opted for a “Live Aid” model where sessions will be spread across time zones to reflect the membership. We don’t expect everyone to attend all the talks given the time differences although you will see me in my pyjamas trying to! The meeting will be free to all members of the society and we hope in particular it will provide a mechanism for final year PhD students to still present their work in a year where travel will be severely limited.

Membership brings me on to another subject. We really need you to register as members of the Society’s (<http://metabolomicsociety.org/members-center/membership>) so you can take part in the Society’s elections. The electorate consists of all full members of the society and this year we have a number of directors either completing their terms or up for re-election. Also, this year we need new officers as Nichole, Krista and I will stand down after completing our maximum terms. While this year has been a bruising one, the officer roles are immensely rewarding and thanks to the careful stewardship of Nichole, we will pass on a society in good financial shape despite the recent events. If you are lucky to be young enough, there are also elections for the EMN. I encourage you all to consider standing for positions within the society and look forward to brighter days with you all!

Dr. Julian Griffin



## Dr. Fidele Tugizimana

### Research Scientist

International R&D division, Omnia Group, Ltd  
Department of Biochemistry,  
University of Johannesburg,  
South Africa

### Short Biography

Originally from Rwanda (and currently living in South Africa, SA), Dr. Fidele Tugizimana holds a B.Phil. in Philosophy (Urbaniana University, Rome-Italy), B.Sc. in Biochemistry-Chemistry (University of Johannesburg / UJ, SA), B.Sc. Hons. in Biochemistry (UJ), M.Sc. and Ph.D. in Biochemistry (UJ). He has received different non-degree purpose training in Advanced Mathematics (UNISA), in Metabolomics for Life Sciences (EMBO, Cambridge, UK) and in Metabolic modelling, Pathway and Flux analyses (Wageningen University, Netherlands).

He is currently a specialist scientist in the International R&D management of the Omnia Group Ltd. SA, a research scientist in the Department of Biochemistry at UJ, a scientific consultant in the L.E.A.F. Pharmaceuticals LLC company (USA & Rwanda) and an advisor in the Rwandan Ministry of Health.

Dr. Tugizimana applies metabolomics approaches in interrogating cellular biochemistry at a global level, specifically in plant-environment interactions and in natural products research. His research contribution has been to elucidate biochemical and molecular mechanisms governing the

responses of naïve and primed plants to biotic or abiotic stresses, and in biostimulant-plant interactions. He has also made contributions in the development of methodologies in metabolomics data acquisition and analysis and in mass-spectrometry-based metabolite identification.

He is an active member of SA scientific societies, the International Metabolomics Society (as a member of different committees and task groups), and the President/Chairperson of Metabolomics South Africa (MSA), an affiliate to the International Metabolomics Society. Dr. Tugizimana (young scientist) is an author/co-author of several metabolomics papers in leading peer-reviewed international scientific journals; and he serves as a guest editor and a reviewer for international scientific journals such as *Metabolomics*, *Frontiers in Plant Science*, *Molecules*, *Metabolites* and *Nature Scientific Reports*.

## Interview Q&A

### How did you get involved in metabolomics?

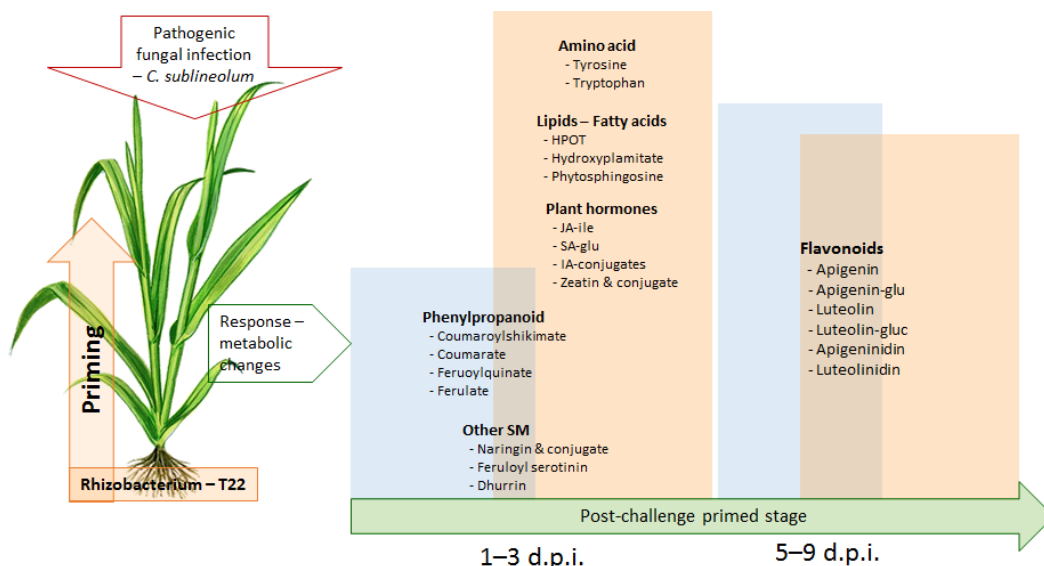
My involvement in metabolomics started a decade ago, when I worked on a mini-research project consisting of profiling defense-related secondary metabolites in tobacco cell suspensions treated with a fungal-derived PAMP molecule. As I dived into the literature and learning journey about metabolomics, I got enthusiastically captivated by different aspects of the metabolomics workflow: the instrumentation (particularly mass spectrometry), the chemistry and data mining. Furthermore, seeing the biochemical insights gained through metabolomics was really motivational and exciting. I should mention that throughout this journey, I got a chance to encounter people in the metabolomics community, who indeed had an impact on my 'love of metabolomics', with some of whom we are now collaborating in different ways: Reza Salek and Fabien Jourdan (at the 2012 EMBO metabolomics workshop, Cambridge, UK), Jacques Vervoorte and Robert Hall (at the Wageningen University, Netherlands), Justin van der Hooft and Karl Burgess.

Since 2016, I became actively involved in the Metabolomics Society activities in different committees and task groups: the EMN Committee, Society Strategy Task Group, Data Standards Task Group and the international organizing committee for the annual metabolomics conference. Furthermore, since 2015, I have been involved in metabolomics training in South Africa and an active member of the newly established Metabolomics South Africa (MSA).

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

Over the last few years, I've been applying metabolomics to interrogate cellular biochemistry, particularly in plant-environment systems; elucidating hypothetical frameworks that describe key biochemical processes and molecular mechanisms involved in plant responses to environmental constraints (abiotic and biotic) [1,2]. It is indeed fascinating to illuminate the complexities and dynamics of the plant's chemical and molecular space in the context of plant-environment interactions, decoding key metabolic profiles and circuits that define the biochemistry of the (naïve or primed) plant defenseome (see the Figure below).

In addition to plant systems, driven by the enthusiasm of biochemical insights discovered through metabolomics, I collaborate with colleagues who apply metabolomics in human infectious diseases research, such as HIV [3] and in the field of food processing [4]. Furthermore, being interested in contributing to the growth of the metabolomics field, with interests in harnessing metabolomics data (from data generation to interpretation), I've been involved in conversations towards the efforts to improve some of the fundamental aspects in metabolomics data: e.g., the effects of ESI parameters in data acquisition [5]; impacts of data processing parameters on model qualities; and collaborating with Dr. Madala on MS-based annotation: exploring fragmentation patterns for (differential) structural elucidation.



**Figure:** A schematic diagram of comparative metabolic changes in PGPR primed and naïve sorghum plants during a post-challenge stage with a hemibiotrophic fungal pathogen. Blue = naïve plants and orange = primed plants [6].



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

Currently I work in the international R&D management division of the South Africa-based multinational company, Omnia Group, Ltd, where I apply metabolomics in the company's agricultural involvement sector. I'm also a research scientist in the Department of Biochemistry at the University of Johannesburg (SA), where the metabolomics research comprises two application areas: human metabolomics – characterization of infectious diseases such as HIV/AIDS, HIV-associated comorbidities and elucidating treatment response mechanisms (driven by Lungile Sitole); and plant metabolomics (where I'm mainly involved) – investigating the biochemistry that defines the interactions between (naïve and/or primed) crop plants and the environment. One of the plant metabolomics research aspects that we are working on is to understand the chemical intercommunications between rhizobacteria and crop plants, and the resultant biochemical events that lead to enhanced growth promotion and defense responses against adverse environmental conditions. Besides, the metabolomics applications in the fields I mentioned, I have been involved in driving the implementation of tools and workflows used in extracting information from metabolomics data. Currently I am interested in exploring the use of machine learning algorithms (and DL) in data mining, and the use of integrated (novel) computational tools (e.g., GNPS, MS2LDA, etc.) to illuminate the MS-captured molecular universe of plant systems. I have no doubt these tools and resources will aid immensely in gaining more biochemical insights, enabling us to understand and discover fundamental knowledge thereof.

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

The metabolomics community in South Africa comprises growing world-class research centers, groups and facilities that are diverse in their research focus: contribution to metabolomics methodologies, and application of metabolomics in plant sciences, infectious disease (such as HIV and TB) and cancer research. In 2018, Metabolomics South Africa (MSA, [www.metabolomics-sa.co.za](http://www.metabolomics-sa.co.za)) was formed; and as of July 2018, MSA is an International Affiliate of the Metabolomics Society with shared goals and mission in advancing the field of metabolomics. The mission of MSA is to promote the growth and development of the field of metabolomics, particularly in South Africa (and, by extension, in Africa). This association is initially established to improve the profile of metabolomics research and technology in South Africa and to foster networking, training, information sharing, mentoring, and career opportunities. The MSA membership is growing exponentially, with more than 150 members, which is an indication of the growing momentum and interest in the field of metabolomics in South Africa. The MSA, in partnership with the African Center of Gene

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

Three aspects to mention: (i) applying metabolomics (with integration of other omics approaches) in decoding biochemical and molecular mechanisms describing the phenomenology of plant-environment interactions (particularly primed and naïve plants, responding to (a) biotic stresses) is a necessary step, providing key fundamental knowledge and understanding required to devise and explore novel strategies for improved crop health and resilience in a changing climate – a typical example here would be my current work at Omnia, as mentioned above; (ii) the exploration and application of machine learning methods (classical and novel) in mining metabolomics data, maximizing the value of untargeted metabolomics data; (iii) metabolite annotation – exploring MS capabilities in collecting spectral information for structural elucidation, and emerging computational tools and resources for biological interpretation of metabolomics data.

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

Speaking from the perspective of someone who applies metabolomics to elucidate the biochemistry of biological systems, metabolomics has disruptively positioned itself as one of the central pillars in systems biology, and has increased in popularity and applicability across a vast array of fundamental and translational research domains. The metabolome, carrying imprints of genetic and environmental factors, decoding metabolic profiles, networks and fluxes, provides one of the best ways to describe metabolism as accurately and precisely as we currently can. Furthermore, the multidisciplinary nature of metabolomics makes it a fascinating but demanding field, with great opportunities. Metabolomics not only brings together different skill sets such as chemistry, biology, computer science and data analytics, but feedback arising from the growth, challenges and applicability of the field also contributes in shaping these disciplines. For instance, one can look at recent technological advancements in analytical platforms (e.g., in MS and NMR for improved measurement of small molecules) and increasing computational and bioinformatics resources.

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

Metabolomics is now a well-established and rapidly developing field. Despite its maturity, there are still some bottlenecks indeed, which affect metabolomics-derived insights. These challenges and barriers include metabolite annotation and identification, correct reporting, big data analytics tools and data sharing. At the same time, one should appreciate ongoing efforts and conversations (in the metabolomics community) to continuously address such barriers. As mentioned, computational tools and workflows that are being developed and promoted (e.g., GNPS, MS2LDA, SMART-NMR, etc.) are indeed improving the characterization and decoding of the molecular/metabolite space; the exploration and use of deep learning methods will indeed aid in mining the increasingly big and complex metabolomics data; and cloud metabolomics initiatives and the insistence and invitation to scientists in the field to share their data, etc.

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

There are increasingly advancements that are continuously shaping and positioning metabolomics in the current, modern science and global reality – the dawn of a new era shaped by the fourth industrial revolution (4IR) philosophy. We see already technological developments, with newer generations in instrumentation, equipped with analytical intelligence and technological capabilities of high-resolution, high sensitivity and high-throughput [7–9]. Furthermore, there are cutting-edge, multi-platform centers (phenome centers and integrated-omics research centers) that are already a reality, with great (potential) impact. However, I would still mention some areas in which efforts are still needed, and these include (i) metabolite identification, (ii) spatially- and time-resolved metabolomics, (iii) integration of metabolomics with other omics, (iv) involvement of machine learning/deep learning methods in data mining and interpretation and (v) training. This last point, training in metabolomics, is still an imperative need for the growth and promotion of metabolomics, globally. I would like to also point out some of the aspects expressed in the recent membership survey conducted by the Metabolomics Society and the Strategy Task Group: support of the early-career members of the Society and promotion of members networking, which surely will (would) impact the membership and also the science [10].

### What role can metabolomics standards play?

Standardization is essential and critical for any scientific field. Metabolomics standards initiatives provide minimum guidelines for conducting and reporting on different aspects of a metabolomics study. Surely such standardization is improved as the field grows and matures, with advancement in technology. There are different scientific task groups of the Metabolomics Society (see under the Society website, under Board & Committees), that are formed to continuously build consensus on reporting standards, for best practices and scientific rigor, necessary for accurate scientific inquiry and knowledge generation. For instance, recently, the Metabolomics Society and the Metabolite Identification Task Group sent out a call for the community to provide feedback on revised reporting standards for metabolite annotation/identification.

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

I have fallen in love with the field of metabolomics and this love keeps growing bigger and stronger every year. As a multidisciplinary field, metabolomics brings an excitement of collaborative nature – interacting with other scientists from different disciplines. And I believe, with continuously increasing developments and community efforts and networking, metabolomics will keep redefining and repositioning itself (in this evolution of human reality), and contributing in knowledge generation, with transforming impacts.

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# Recent Publications

Recently published papers in metabolomics

- [Milk Metabotyping Identifies Metabolite Alterations in the Whole Raw Milk of Dairy Cows with Lameness](#)
- [A High-Performing Plasma Metabolite Panel for Early-Stage Lung Cancer Detection.](#)
- [Single-Cell Metabolic Profiling: Metabolite Formulas from Isotopic Fine Structures in Heterogeneous Plant Cell Populations.](#)
- [Exploring feature selection of St John's wort grown under different light spectra using <sup>1</sup>H-NMR spectroscopy.](#)
- [Toxicometabolomics of the new psychoactive substances -PBP and -PEP studied in HepaRG cell incubates by means of untargeted metabolomics revealed unexpected amino acid adducts.](#)
- [Signaling lipids as diagnostic biomarkers for ocular surface cicatrizing conjunctivitis.](#)
- [A fungal pathogen induces systemic susceptibility and systemic shifts in wheat metabolome and microbiome composition.](#)
- [Dried blood spot-based metabolomic profiling in adults with cystic fibrosis.](#)
- [Authenticity and quality evaluation of different Rhodiola species and commercial products based on NMR-spectroscopy and HPLC.](#)
- [Circulating plasma metabolites and risk of rheumatoid arthritis in the Nurses' Health Study.](#)
- [BioHackathon 2015: Semantics of data for life sciences and reproducible research.](#)
- [Molecular networks in Network Medicine: Development and applications.](#)



# Metabolomics Events

6-10 Jul 2020

Metabolomics 2020

**Venue**

Virtual Meeting

The 16th Annual International Conference of the Metabolomics Society was scheduled to be held in Shanghai, China in July 2020. Due to COVID-19 concerns, the in-person meeting has been cancelled for 2020 and a virtual meeting will take place instead. Check back for updates in the coming weeks at <http://metabolomics2020.org>.

6-10 Jul 2020

Introduction to Nutritional Metabolomics

**Venue**

Department of Nutrition Exercise and Sports, University of Copenhagen, Denmark

**Overview**

The course will provide an overview of LC-MS based untargeted metabolomics and its application in nutrition. It will be delivered using a mixture of lectures, hands-on data preparation and analysis, computer-based practical sessions, and discussions. Visits to wet labs and instructions on human sample preparation procedures is included but with minimal hands-on.

The students will go through common steps in a typical metabolomics study using a real-life case. This case study includes collected plasma (or urine) samples from a nutritional intervention. The sample preparation and analysis on UPLC-QTOF has been conducted and the students will further process and analyse the acquired data with various freeware tools (e.g., R, XCMS, MZmine and MetaboAnalyst). They will finally work on identification of relevant metabolites using several web-based structure elucidation tools. The course will conclude by presentations of reports generated by the students based on the case study.

## Metabolomics Events

The course will be structured as initial short lectures on theory followed by hands-on exercises, which will teach the students to transfer the theoretical information to practice.

### Fee

No fee for the PhD students under the Open Market in Denmark and NOVA partners.

Other participants are to pay a course fee of 300 EUR. Each student must pay and arrange their own travel and accommodation in Copenhagen during the course.

### Course link

<https://phdcourses.ku.dk/detailkursus.aspx?id=107283&sitepath=NAT>

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## 15 Jul 2020

### ISMB 2020 CompMS – Save the date & call for proposals

#### Venue

Palais des congrès de Montréal, Montreal, Canada

Please join us during the ISMB 2020 conference for the Computational Mass Spectrometry (CompMS) COSI session on July 15, 2020 in Montreal, Canada.

The ISMB conference is the world's largest bioinformatics/computational biology conference. Every year it brings together scientists from computer science, molecular biology, mathematics, statistics, and related fields and provides an intense multidisciplinary forum for disseminating the latest developments in bioinformatics/computational biology. The conference fosters fresh dialogues, collaboration and learning opportunities, and is a gathering which shapes the future of the field.

At the heart of the scientific program are ISCB's Communities of Special Interest (COSIs), enabling community involvement and bolstering ISMB's reputation as the leading conference in the field. The CompMS COSI promotes the efficient, high quality analysis of mass spectrometry data through dissemination and training in existing approaches and discussion of new, innovative approaches. The CompMS initiative aims to exploit synergies between different application domains, in particular proteomics and metabolomics.

A strong scientific and technical program showcases the best international developments in bioinformatics and computational biology, making ISMB 2020 a must attend event.

Date: July 15, 2020 (CompMS COSI) / July 13–16, 2020 (ISMB)

#### Conference link

<https://www.iscb.org/ismb2020>

## Metabolomics Events

### 24 Jul 2020

#### Cancer and Immuno-Metabolism Symposium

##### Venue

University of Kentucky's Center for Environmental & Systems Biochemistry

##### Overview

Hear and meet researchers who use stable isotope labeling and other approaches to investigate metabolism in many physiological systems – such as immune cells, cancers and brain metabolism. Poster sessions and exhibitors will offer additional learning and networking opportunities.

For more information, contact Alicia Colliver at: [ajduna0@uky.edu](mailto:ajduna0@uky.edu)

View details [here](#).

### 14-16 Sep 2020

#### Metabolomics Association of North America (MANA) 2nd Annual MANA Conference

##### Venue:

Online

##### Confirmed speakers

- Joshua Rabinowitz, Princeton University
- Nima Sharifi, Cleveland Clinic
- Charles Serhan, Harvard University
- Wassim Labaki, University of Michigan
- Ian Lewis, University of Calgary

##### Overview

The conference will feature oral presentations, poster sessions and interactive forums with live discussion of key challenges in different metabolomics subfields.

**Abstract submission deadline: July 17, 2020**

##### Course link

Information and registration: <https://www.mana2020.org>

## 23-25 Sep 2020

### Multiple Biofluid and Tissue Types, From Sample Preparation to Analysis Strategies for Metabolomics

#### Venue:

Birmingham Metabolomics Training Centre, University of Birmingham, United Kingdom

#### Overview

This 3-day course provides a theoretical overview and hands-on training to apply multiple sample preparation and UPLC-MS methods to characterise the metabolomes of complex biological samples using the mass spectrometer (Xevo QToF G2-XS - a maximum of 4 people working on the instrument in a session). The course is led by experts in the field who have experience of the analysis of microbial, plant and mammalian samples, and illustrates the different approaches that are available to analyse a range of biological samples and applying complementary liquid chromatography approaches to maximise the coverage of the metabolome.

#### Topics covered

- Introduction to dealing with the complexity of biological samples using UPLC-MS
- Overview of different sample collection, sample quenching and sample extraction methods
- The challenges of working with cellular and tissue samples
- Overview of different UPLC methods including HILIC and reversed phase methods
- Hands-on sample preparation of plasma, urine, cell and tissue samples
- Monophasic and biphasic solvent extraction methods to target polar and non-polar metabolites
- SPE and liquid-liquid sample clean-up methods
- Hands-on HILIC and reversed-phase liquid chromatography
- Hands-on UPLC-MS analysis for untargeted studies (maximum of 4 people)
- Overview of data analysis and metabolite identification
- Problem solving and tips and tricks session with the experts

#### Course link

More information available [here](#).



## 7-9 Oct 2020

### Introduction to Metabolomics for the Microbiologist

#### Venue

Birmingham Metabolomics Training Centre, University of Birmingham, United Kingdom

#### Overview

This three-day course introduces how untargeted metabolomics can be applied to study microbial systems in academic and industrial research. The course provides an overview of the metabolomics pipeline, experimental design, sample preparation and data acquisition. The course is led by experts in the field of metabolomics and will include lectures, hands-on laboratory sessions in sample preparation and data acquisition and computer workshops focused on data processing and data analysis.

#### Topics Covered

- Introduction to metabolomics, both targeted and untargeted approaches
- Experimental design and the importance of quality control samples in untargeted metabolomics
- Analytical strategies applied in metabolomics with a focus on mass spectrometry
- Hands-on laboratory sessions focused on sample preparation and to include metabolic quenching and extraction procedures, intracellular and exometabolome samples and polar and non-polar extraction methods
- Hands-on laboratory sessions focused on sample analysis for untargeted metabolomics studies using an Acquity UPLC coupled to a Xevo QToF mass spectrometer
- Hands-on workshop focused on data processing and data analysis
- Hands-on workshop focused on an introduction to metabolite identification
- Question and answer session with the experts

#### Course link

More information available [here](#).

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## 26-27 Oct 2020

### Targeting CNS Tumor Metabolism Symposium

#### Venue

NIH Campus, Bethesda, Maryland

#### Overview

This is the first conference that focuses on the tumor metabolism and it is expected to be a didactic and collegial learning environment. Metabolic investigations for these tumors have been conducted in isolation and the goal of this meeting is to bring together the clinicians with the experts in metabolism to increase the utilization of metabolic investigations in the clinical settings. This will, in turn, enhance partnerships and advance the treatment for patients.

In addition to oral and poster presentations selected from the submitted abstracts, the conference will feature invited lectures from an internationally recognized faculty, including keynote talks from Craig Thompson, MD (President and CEO of Memorial Sloan Kettering Cancer Center) and Paul Mischel, MD (Distinguished Professor, University of California San Diego).

**Abstract submission deadline is Monday, June 15, 2020, 11:59pm CST.**

#### Course link

<https://www.soc-neuro-onc.org/SNO/2020METAB/Home.aspx>

**2-4 Nov 2020**

### Metabolomics with the Q Exactive

#### Venue

Birmingham Metabolomics Training Centre, University of Birmingham, United Kingdom

#### Overview

This 3-day course introduces you to using the Q Exactive mass spectrometer in your metabolomics investigations. The course is led by experts in the field of metabolomics and includes lectures, laboratory sessions and computer workshops to provide a detailed overview of the metabolomics pipeline applying the Q Exactive mass spectrometer.

#### Topics covered

- Introduction to Metabolomics on the Q Exactive, the metabolomics workflow, and case studies using the Q Exactive
- Using the Q Exactive family of instruments in your metabolomics investigations
- Experimental design and the importance of quality control samples
- Sample preparation including polar and non-polar preparation methods on biofluids (urine and plasma) and tissue samples
- Preparation of samples for profiling and targeted analyses on the Q Exactive
- Hands-on data acquisition for profiling and targeted studies, setting up the Vanquish UHPLC coupled to the Q Exactive MS
- Data processing workshop
- Data analysis workshop (univariate and multivariate analysis)
- Introduction to metabolite identification applying Data Dependent Analysis and Data Independent Analysis
- Question and answer session with a panel of experts
- Tips and tricks
- Problem solving

#### Course link

More information available [here](#).

## 5-6 Nov 2020

### Metabolite identification with the Q Exactive and LTQ Orbitrap

#### Venue

Birmingham Metabolomics Training Centre, University of Birmingham, United Kingdom

#### Overview

This 2-day course will provide a hands-on approach to teach the attendees about the latest techniques and tools available to perform metabolite identification in non-targeted metabolomics studies. The course will be led by experts working within the fields of metabolomics and chemical analysis and will include a significant proportion of hands-on experience of using mass spectrometers, software tools and databases. A maximum of four people will be working on each mass spectrometer in a session. We will apply these tools on the Q Exactive and LTQ-Orbitrap family of mass spectrometers.

#### Topics Covered

- Importance of mass spectral interpretation
- Types of data which can be collected on the QE and LTQ-Orbitrap (m/z, retention time, MS/MS, MS<sup>n</sup>)
- Conversion of raw data to molecular formula and putative metabolite annotations
- MS/MS experiments in metabolic phenotyping for on-line data acquisition using the QE (DDA, DIA, all-ion)

#### Topics Covered

- MS/MS and MS<sup>n</sup> experiments for sample fractions using the LTQ-Orbitrap
- Mass spectral libraries (using mzCloud)
- Searching mass spectral libraries
- Tools for mass spectral interpretation
- Reporting standards for metabolite identification
- Question and answer session with the experts

#### Course link

More information available [here](#).

## Postponed Until 2021

### The Third Annual Canadian Metabolomics Conference

**Venue:**

Edmonton, Alberta, Canada

**Overview**

The Third Annual Canadian Metabolomics Conference has been postponed until 2021. The conference will highlight work by leading researchers, including new technologies and approaches for metabolomics research, and applications in various fields. The conference will feature networking opportunities and a poster session designed for trainees to present their work. Our goal is to highlight the exceptional metabolomics science that is being done in Canada and abroad, and foster Canada's leadership role in the global research community.

We look forward to seeing you in 2021!

**Conference link**

<https://www.canmetcon.ca/>

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## 15-16 Apr 2021

### Data analysis for Metabolomics

**Venue**

Wageningen Campus, The Netherlands

**Overview**

Event postponed from June 4-5, 2020 to now April 15-16, 2021

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.

**Course link**

<https://www.wur.nl/en/Education-Programmes/Wageningen-Academy/Plant/Course-Data-analysis-for-Metabolomics.htm>

# Metabolomics Jobs & Collaborations

If you have a job you would like posted, please email Shelby Soke ([soke@ualberta.ca](mailto:soke@ualberta.ca)).

## Jobs Offered

Job Title	Employer	Location	Posted	Closes	Source
Postdoctoral researcher	iDiv, Ecometer	Leipzig, Germany	May 2020	26-Jun-20	<a href="#">iDiv</a>
Technician	iDiv, Molecular Interaction Ecology	Leipzig, Germany	May 2020	26-Jun-20	<a href="#">iDiv</a>
Early Stage Researcher (Marie Curie Fellow)	Queen's University Belfast	Belfast, Northern Ireland, UK	May 2020	10th July 2020 4pm UTC	<a href="https://www.qub.ac.uk/Study/">https://www.qub.ac.uk/Study/</a>
Various positions			27-May-20		<a href="#">Metabolomics Association of North America Jobs</a>
Are you a skilled metabolomics expert/ analytical chemist?	MS-Omics	Vedbaek/ Copenhagen, Denmark	26-May-20	1-Sep-20	<a href="#">Metabolomics Society Jobs</a>
Postdoctoral Researcher in Metabolomics/ Computational Metabolomics	Institute for Biomedicine, Eurac Research	Bolzano, Italy	13-May-20	Until filled	<a href="#">Metabolomics Society Jobs</a>
Postdoctoral Fellowship in MALDI Imaging Mass Spectrometry	U.S. Food and Drug Administration	Jefferson, Arkansas, USA	6-May-20	Until filled	<a href="#">Metabolomics Society Jobs</a>
Research Postdoctoral Scientist	Beaumont Health (Metabolomics Department)	Royal Oak, Michigan, USA	29-Feb-20	Until filled	<a href="#">MetaboNews Jobs</a>
Postdoctoral Research Fellow in Microbial Metabolomics and Natural Products Chemistry	Fundación MEDINA	Granada, Spain	21-Feb-20	Until filled	<a href="#">Fundación MEDINA</a>
Postdoctoral Associate	Yale School of Public Health	New Haven, Connecticut	5-Feb-20	Until filled	<a href="#">Metabolomics Society Jobs</a>
Senior Bioinformatician	Ann & Robert H Lurie Children's Hospital	Chicago, Illinois, USA	16-Jan-20	Until filled	<a href="#">Ann &amp; Robert H Lurie Children's Hospital</a>
Two Postdoctoral Fellowships	Università Cattolica del Sacro Cuore	Piacenza, Italy	8-Jan-20		<a href="#">MetaboNews Jobs</a>

June 2020

## Metabolomics Jobs

# 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 Shelby Soke ([soke@ualberta.ca](mailto:soke@ualberta.ca)). Upon review, a limited number of job submissions will be selected for publication in the Jobs Wanted section.

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