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MetaboNews

This month in metabolomics

October, 2024 Vol 14, Issue 10

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





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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

Conference Corner

Save the Date!

We hope to see you in Prague next year, from June 22 – 26, 2025. Mark your calendar and keep an eye out for updates regarding sponsorship packages and



registration. The deadline for abstracts will be earlier this year, in February, so plan ahead to present your latest findings with us in Prague!

Members' Corner

Board of Directors - Words from The Chair Warwick Dunn

Dear Metabolomics Society Members and metabolomics friends,

It is very humbling as well as a great honour and privilege to be able to write this first

message to you as President of the Metabolomics Society. The Metabolomics Society and community as a whole are very close to my heart, and I look forward to serving the Society and you over the next two years. I have worked with the Society from 2009 in different roles and hope to continue serving the Society after the next two years.

I would like to thank our past-president (Roy Goodacre) and past-secretary (Fabien Jourdan) for their significant work to support the society over recent years and for ensuring that the society is in excellent shape moving forward. Their workload was significant, voluntary and mostly behind the scenes. Importantly, our past-president sits three offices down the corridor in Liverpool and so will always be available for advice and support.

Each Director of the Metabolomics Society can serve two terms of normally two years for each term. In the elections over the summer we welcomed Elizabeth Want, Aurelia Williams and Nicholas Rattray to the Board of Directors – welcome all. Maria Eugenia Monge, Tomáš Pluskal and Lynn Vanhaecke were re-elected for a second term. I am looking forward to working with Maria (Secretary), Candice Ulmer Holland (Treasurer) and all of the Directors over the next two years to help drive forward the society to represent the metabolomics community globally.

I will keep you updated as we move forward and look forward to meeting you at our annual conferences.

All the very best,

Warwick (Rick) Dunn, University of Liverpool, UK President, Metabolomics Society



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Early-Career Members Network (EMN)

EMN Elections

EMN 2024-2025 committee kicked off in October 2024, with a strong representation across the globe. EMN is happy to announce Breanna Dixon has been elected as the new treasurer of EMN, while Monique Ryan has been elected as the new secretary. Silvia Radenkovic will continue as the EMN chair. The EMN committee would also like to welcome again our new committee members, Ambrin Farizah Babu, Marina Tonetti Botana, Thomas Dussarrat, Loic Mervant, and Jayden Lee Roberts.



ECR Voices 2024-2025

The EMN 'ECR Voices' initiative to spotlight early-career researchers (PhD students, Postdocs, Young Investigators, etc.) on our Twitter/X account is continuing through 2024-2025! You can check out an example here:

(https://x.com/EMN_MetSoc/status/1704787637591265456?s=20). We encourage everyone to participate! You can easily create your own ECR Voice slide using this link: (https://docs.google.com/presentation/d/1H43FIIp3gmtJMUYS6r-

<u>2XVd460N8PjBn/edit#slide=id.p15</u>). The link contains instructions, templates, and examples from other researchers already featured on our Twitter/X page. It's as simple as making a single PowerPoint slide with a headshot and a few bullet points about yourself! Please consider sharing ECR voices with your network! This year, we would like to invite the researchers especially from South America, Africa and Asia to participate. If you are interested, or want to recommend someone from your network, please reach out to info.emn@metabolomicssociety.org.

Task Group Corner

International Affiliations Task Group

Affiliates Training Network is established. The network aims to facilitate training, research visits and short (3-6 month) exchanges of young scientists across the labs from affiliated societies. As initial steps, the network will

- establish initial lists of laboratories interested to host students from abroad (regions of other Affiliates), with potential commitment to contribute to financing of such exchange;
- exchange information about current training and exchange opportunities for students from abroad;
- together with the Metabolomics Society, consider how the affiliates could contribute
 to financial support of the network. As part of this network, at least one of the
 affiliates is currently already planning to open 2-3 student exchanges with own
 financing.

International Affiliates' Corner

Australia & New Zealand Metabolomics Society (ANZMetSoc)

Visit https://anzmetabolomics.org/what-we-do

AUS-oMicS 2025 - Registrations open!

We're thrilled to announce that the registration portal for **AUS-oMicS 2025** is officially open!

Get ready to join us in beautiful Cairns, Queensland, Australia, from <u>May 18 - 21, 2025</u>, for an unforgettable event. We can't wait to see you there!

Conference website: https://www.ausomics.com/

Register Now for Early Bird Prices: https://www.ausomics.com/registration1

The Conference has secured several discounted Hilton Cairns and Pullman Hotels rooms.

Book today via the registration and save! Secure Accommodation here: https://www.ausomics.com/accommodation

Réseau Français de Métabolomique et Fluxomique (RFMF)

Visit http://www.rfmf.fr/



17th RFMF meeting in Paris, France

The 17th edition of the French Speaking Network of Metabolomics and Fluxomics (RFMF) Scientific Days will be held in the heart of Paris, in the Saint-Germain-des-Prés district from June 10 to 13. This iconic Parisian cultural hub, located in the 6th arrondissement, originated with the founding of the Abbey of Saint Vincent in 543, later renamed Saint-Germain-des-Prés in the 7th century. Its intellectual and spiritual influence shaped the historic Saint Germain district. From the 17th century, fairs and markets introduced shows that inspired modern boulevard theatre. This mix of intellectual, commercial, and artistic life created the district's unique character, where creatives and shoppers mingle. After the Revolution, it remained a cultural centre, known for its cafés, literary prizes, and vibrant jazz scene since the 1950s.

The upcoming RFMF meeting will once again offer a valuable opportunity for our vibrant community to come together and share ideas. The event will include several plenary lectures from internationally acclaimed researchers, along with oral presentations, flash talks, and poster sessions. Continuing the tradition from recent meetings, some oral presentation slots will be reserved for showcasing the work of young researchers in the field. Additionally, the meeting will honour the 2025 thesis prize winner and introduce the newly appointed RFMF honorary member for 2025, who will present a summary of their research.

Book the date and we hope to see many of you there ;)

Metabolomics Association of North America (MANA)



Visit https://metabolomicsna.org
email mana@metabolomicsna.org

LinkedIn @MANA (Metabolomics Association of North America)

X <u>@MetabolomicsANA</u>

MANA has launched its new MANA membership system! You can become a member by visiting the MANA website (metabolomics.org) and clicking "Become a Member" on top right-hand side of our home page. It only takes 5 minutes! After November, you will stop receiving our mailings unless you are have renewed your MANA membership. Join or renew now to make sure you don't miss future updates!

The following nominations are also open:

- 4 positions on MANA board of directors: nominations are due by 11 pm EST on Oct 29; please use the following URL to submit nominations: https://forms.gle/shim\Wu4D87eKpReA
- 5 positions on the Early Career Member Council: nominations are due on November 8th, 2024; please use this link for more information: https://bit.ly/MANA-ECM-Elections.

As always, remember to visit our <u>website</u> for the latest and remember to also visit <u>our job board</u> for open positions in metabolomics.

Scottish Metabolomics Society

Visit http://www.scottishmetabolomics.net/

Establishment of the SMN Technical Forum

On the 4th of October the SMN hosted its first Technical Forum where 15 researchers from across Scotland met online to discuss a range of 'live' research problems. The aim of the forum is to provide a space where technical issues related to ongoing metabolomics experiments can be discussed and draw upon the collective expertise of the community to solve them. The next meeting will take place in November and all comers are welcome (see SMN on Twitter and LinkedIn for upcoming details).

Scottish Metabolomics Network Annual Symposium

Visit: http://scottishmetabolomics.net/

Over 100 researchers are signed up to the Scottish Metabolomics Network al symposium that will be hosted on the 22nd and 23rd of October 2024 within the Institute of Aquaculture at the University of Stirling, late comers are welcome! There will be a range of talks and posters on all aspects of metabolomics and local and international metabolomics researchers are encouraged to visit Stirling and experience its rich medieval history and stunning scenery. On the Monday before the event (21st) there will also be a hands-on chemometrics training workshop aim at developing stats skills for ECRs.

The conference will include plenary sessions from Professor Paul Fraser from Royal Holloway University of London and Dr Thierry Schmidlin from the University of Mainz.



Thailand Metabolomics Society (TMS)

Visit https://thailand-metabolomics.org/

The 2nd Thailand Metabolomics Society Conference: Rise of Metabolomics in Thailand

The 2nd Thailand Metabolomics Society (TMS) Conference was held on October 3-4, 2024, at K Building, Vidyasirimedhi Institute of Science and Technology (VISTEC) in Rayong, Thailand. The theme of this year's conference was "Rise of Metabolomics in Thailand." The event was organized by prominent Thai universities and research institutions, including VISTEC, Mahidol University, Khon Kaen University, Chulalongkorn University, the National Center for Genetic Engineering and Biotechnology (BIOTEC), Kasetsart University, and Prince of Songkla University.

The goals of the conference were to advance metabolomics research and promote knowledge sharing and collaboration among national and international institutions. The two-day program included short courses on sample preparation, a metabolomics workshop, and presentations on recent metabolomics research in Thailand. Topics covered six major areas: environmental metabolomics, food and nutrition, plant

metabolomics, biotechnology, natural products (including pharmaceuticals and host-microbe interactions), and clinical metabolomics.

The conference commenced with opening remarks from Prof. Dr. Yongyut Sirivatanauksorn and Dr. Wonnop Visessanguan, President and Vice President of TMS, respectively. There were eleven invited speakers who presented their research, complemented by 33 poster presentations from students and researchers. A plenary session was led by Prof. Dr. Pimchai Chaiyen, President of VISTEC, focusing on "Insights into Synthetic Cells through Metabolomics."

Invited Speakers:

- Dr. Sahutchai Inwongwan: The Impact of PM2.5 from Northern Thailand on Lung Cancer Progression: A Multi-Omics Approach
- Dr. Atikorn Panya: Flavor-Sensomics at NSTDA: A Closer Look
- Assoc. Prof. Dr. Supaart Sirikantaramas: From Fruits to Flavors: Metabolomics-Driven Innovations in Plant Research
- Asst. Prof. Dr. Nawaporn Vinayakhin: Untargeted Metabolomics for Probing Bacterial Responses to Environments
- Asst. Prof. Dr. Sivamoke Dissook: Beyond Known Pathways: Metabolomics and the Discovery of Uncharted Biosynthetic Routes
- Prof. Dr. Kornkanok Ingkaninan: Metabolomics in Action: From Herbal Complexity to Standardized Bioactive Ingredients – Case Studies of Brahmi and Teak Extracts
- Assoc. Prof. Dr. Sakda Khoomrung: Advances in Natural Products for Human Health Applications
- Asst. Prof. Dr. Jutarop Phetcharaburanin: Utilizing Global and Targeted
 Metabolomics Combined with Microbiomics for Host-Microbe Crosstalk in Cancer
- Dr. Lucksamon Thamlikitkul: Plasma Metabolomic Analysis in Thai Lung Cancer Patients
- Asst. Prof. Dr. Rossarin Tansawat: Utilizing GC-MS Metabolomics of Breath for Cancer Biomarker Discovery

The conference was sponsored by Agilent Technologies, DKSH, LECO, the Center of Excellence for Innovation in Chemistry (PERCH-CIC), the Computational and Structural Biotechnology Journal (CSBJ), the Ministry of Higher Education, Science, Research and Innovation (MHESI), and the Program Management Unit for Human Resources & Institutional Development, Research and Innovation (PMU-B).

The 2nd Thailand Metabolomics Society Conference was successful in providing a platform for national researchers to connect, engage in meaningful discussions, and foster collaborations among researchers and institutions. This conference represents a vital step

toward advancing metabolomics research in Thailand.



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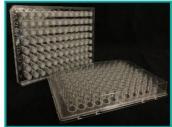
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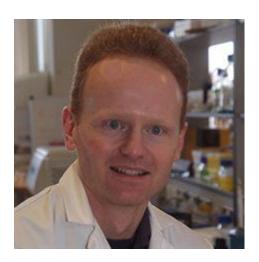
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MetaboInterview

Dr. Mark Viant



Dr. Mark Viant

Professor of Metabolomics at the University of Birmingham

Co-founder & CEO of Michabo Health Science Ltd

Biography

Professor Viant completed a BSc in Chemistry (1991) and a PhD in Chemical Physics (1994) at the University of Southampton, UK. He then spent nearly a decade in the USA, first as a Royal Commission for the Exhibition of 1851 Postdoctoral Researcher at the University of California - Berkeley and later as a faculty member at the University of California - Davis, where he pioneered metabolomics in environmental health for aquatic organisms.

In 2003, he joined the <u>University of Birmingham</u> as a NERC Advanced Fellow to develop and apply metabolomics in environmental toxicology. With funding from various agencies, he established a significant research group in environmental metabolomics. He became Reader in Metabolomics in 2008, Director of the NERC Biomolecular Analysis Facility in 2009, and was appointed to his current Chair in 2010. Mark served as President of the Metabolomics Society from 2012 to 2014 and received the Joseph Chamberlain Award for Academic Advancement from the University of Birmingham in 2013. In 2018, alongside his University Chair, he co-founded and became the CEO of <u>Michabo Health Science Ltd</u>.

New Addition: Listen to the responses by clicking on the question

Can you describe the key research initiatives your team is undertaking at the University of Birmingham?

The key research areas focus on the application of metabolomics in toxicology and, more specifically, in regulatory toxicology. I have two teams. One is based in the University of Birmingham, and the other is in a spin-out company from the University. And these two teams collaborate. One has a more academic, basic research focus, while the second team has a more translational and applied focus in regulatory toxicology.

What specific areas of regulatory toxicology is your team focusing on, and what role do you see metabolomics or exposomics in that regulatory landscape?

The team in the university is focusing on underpinning developments to help support and drive forward the use of metabolomics in toxicology. Some specific examples of that include automating sample preparation as this is critical for enabling us to undertake very large scale toxicology studies. This work is done in Phenome Centre Birmingham, and we partner with Beckman Coulter. Also we are developing hybrid LC-MS metabolomics methods that provide both an untargeted measurement of lipids and polar metabolites as well as targeting the new MTox700+ panel, which comprises hundreds of toxicologically relevant metabolites. We conduct some of this work with Thermo Fisher Scientific via a technology partnership.

A third area of research is the simultaneous measurement of both endogenous and xenobiotic compounds in a single assay. Typically, metabolomics is focused on measuring endogenous metabolites and lipids. Over the last few years we have been focused on trying to measure the xenobiotics in biological samples, as well as the endogenous chemicals. Further, not just the xenobiotics themselves, but also to discover and measure the biotransformation products of those xenobiotics. This area of chemical metabolism is really important in toxicology. It's another type of hybrid metabolomics. We published on this in Nature Communications last year.

Another interesting project that we lead in the University is funded by the European Chemicals industry Council (Cefic). The project has industry partners, academic partners, and partners in government, and it's evaluating the reproducibility of metabolomics. In effect an inter laboratory ring trial exercise, but in the context of regulatory toxicology. It's called the MATCHING project, and it's a really nice example of having tripartite perspectives from industry, academia and government labs, seeking to demonstrate the reliability of metabolomics when you apply it to study the effects of chemicals. The project is nearing completion, the results so far are extremely encouraging, with all of the partner labs whose data passed QC having obtained the same toxicological outcome. I think the regulatory toxicology community is quite impressed by metabolomics!

What do you think the biggest impact of your research will be in terms of external impacts? (i.e. day to day experiences or at a policy level?)

We've been building a body of knowledge and continuing to develop our expertise around the use of metabolomics in toxicology for two decades. Consequently I get involved in several expert groups to apply this knowledge, and that provides a route to impact. One project, which was completed and declassified last year, is defining a reporting standard for metabolomics and other omics studies in regulatory toxicology. There's been a lot of standards developed for how you report metabolomics studies over the last two decades. In fact I had the pleasure of being involved in the early MSI work around 2005-2006. The project that we just completed was led by the OECD, and the guidance document that was produced - called the OECD Omics Reporting Framework - is now applicable across all 38 member state countries of the OECD. The impact is clear because of the dissemination of the work internationally. Currently I'm helping to write another OECD guidance document specifically on how you obtain samples for (metabol)omics in regulatory toxicology, whether that be in vitro sampling, in vivo sampling, or using alternative test species. It's using our experience from academia and from the many projects we've undertaken over the last two decades, and then contributing to guidance documents used in the "real world".

What key differences have you noticed between academic research and the startup/spinoff sector? What do you think each could learn from the other?

That's a very interesting question, there are a lot of differences!. Our spin-out was launched in 2018 so I've about six years of business experience versus 20+ years experience in academia. In a spin-out company, the focus is on getting from A to B as rapidly and as effectively as possible, within budget. Project management tools are essential, the work is very directed, and with clear deadlines that you cannot afford to miss. It's adrenaline fuelled! Academia, generally speaking, is not like that. A typical scenario is you've written a proposal for a three year grant which gets approved. When you wrote that proposal you said 'our current knowledge is A and we're going to get to B'. However, by the time you start working on the project, you actually realize that going to C looks more interesting than B, and then while working towards C you make an inadvertent discovery around D!. The space for blue skies innovation is just much greater in a university, because you don't have a deadline almost every other day!. Because of this, I began to regard the university work environment as inefficient compared to the business sector, and in one sense, it really is. But actually, the beauty of research in an academic environment is that it doesn't have the constraint of getting from A to exactly B by a deadline. It has the space for innovation. And so I don't think either should change, both have an exciting role to play. They're just geared to achieve different endpoints.

What are the biggest challenges in interpreting metabolomics data for regulators, and how could we address them?

The worlds of academic metabolomics research and regulatory toxicology are a long way apart, and that makes communication of the science quite challenging. I remember an interesting slide presented by one of my colleagues at the European Commission's Joint Research Center: on the left was "systems biology" - it was a complex network, and was showing the interactions between different metabolites and lipids, the sort of network that an academic would find interesting and dive into wanting to do further data analysis. On the right side of the slide, there was the reality of the chemical regulator's world. The regulator has to decide whether or not a chemical is going to be authorized for use or not. And that is a green or red traffic light. They have a timeline by which that decision has to be made, and they most probably won't have all of the data that they would like to have. So the regulator is working in this data poor space, needing to make a firm and definitive decision by a particular deadline! What's particularly amusing is when you hear an academic reporting on their science discovery. It's almost inevitable that they'll end the interview stating, 'there is a need to do more research, generate more data, to determine a more definitive answer'. So the challenge for us is how to translate from the complex world of multi-dimensional metabolomics to an environment demanding the traffic light is set to green or red. This is a topic we consider a lot in our company, how to convey the key elements of a study that provides the regulator with just the information that they need. Fundamental to understanding that is to deeply understand what the regulator is trying to achieve. As an academic, for many years, I used to think I understood chemical safety regulations. Well I didn't, and it was only after I focused half of my work life on understanding the chemical regulatory problem space, and the laws associated with it, that the communication with the regulators became so much easier. Understanding what is needed from metabolomics within a regulatory context is a key starting point.

If anything, what do you think is a critical issue (technological or otherwise) holding back the wider adoption of metabolomics, especially in how we can translate its impacts to laypeople?

In terms of the critical issues holding back metabolomics, if I was talking purely in an academic sense, I think I would state the same point that you will have seen in many metabolomics interviews over the last decade or so: confident metabolite identification. It's massively progressed but still is a major challenge. If we're thinking in terms of placing metabolomics into a regulated environment, such as chemical safety, then the largest challenge is the requirement for standardization, defining and understanding all the

relevant sources of uncertainties, and making sure that those uncertainties are acceptable within that particular regulated environment.

What advice would you give to researchers interested in transitioning their work from academia to applied settings like regulatory toxicology?

I strongly encourage early-career researchers to think about transitioning metabolomics beyond academia. It is really quite different on the "outside", more than I had envisioned. My key message is if you chose to translate, you need to be really seriously committed to wanting to do it. You're going to have to put a lot of time and energy into doing it. I never had a grand plan for my career to become split equally between academia and business, it evolved like this because I have a passion to use metabolomics in the real-world. Spending half of my week focused on how to translate, and to translate effectively, was necessary in my case. It requires a change in mindset, and a very significant amount of time and effort to do this. Something I did was read a lot of books about startups, including by academics that had stepped outside of academia and gone into business, and about the challenges that they experienced. But it's hugely rewarding! I'm loving this combination of basic research coupled with working in the business sector. Follow your dreams. It is achievable. It's just hard work!

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MetaboReads

This month's papers were selected from a pool of 579, which shows just how busy and exciting our field is. Enjoy this selection of papers - as always, our goal is to bring you some that you've likely heard about, and some you haven't.

- The MetaboNews Team

Metabolomics and Microbiome Interactions in Health and Disease

Metabolomics continues to be a key technology in uncovering host-microbiome interactions,

revealing potential therapeutic targets and strategies. The following papers explore the impact of the microbiome on conditions such as acute myeloid leukemia, transplantation, frailty in the elderly, Alzheimer's disease, and how dietary interventions can modulate these effects

Gut microbiome alterations at acute myeloid leukemia diagnosis are associated with muscle weakness and anorexia

Potgens and colleagues in Haematologica investigated the gut microbiome of antibiotic-free acute myeloid leukemia (AML) patients at diagnosis. They found significant differences in the fecal microbiota composition compared to matched controls, including an increase in oral bacteria and alterations suggesting an altered redox status. Notably, a reduction in Eubacterium eligens was strongly correlated with muscle strength and enterocyte function markers. The study suggests that gut microbiome perturbations in AML patients are associated with muscle weakness and anorexia, highlighting potential therapeutic targets within the microbiome

Prebiotics improve frailty status in community-dwelling older individuals in a double-blind, randomized, controlled trial

Yang and colleagues in the Journal of Clinical Investigation conducted a randomized controlled trial assessing the effects of a prebiotic blend of inulin and oligofructose on frailty in older adults. The intervention significantly improved frailty status, renal function, body composition, walking speed, and grip strength. Metabolomics analyses revealed that prebiotic supplementation modulated the gut microbiota and metabolome, increasing beneficial bacteria and altering metabolic pathways. The findings suggest that prebiotics can modify the gut microbiota to improve frailty status and prevent its progression in the elderly

Dietary fibers boost gut microbiota-produced B vitamin pool and alter host immune landscape

Grant and colleagues in Microbiome examined how different dietary fibers affect the gut microbiota and host immunity in mice. Metabolomics analyses revealed that fiber deprivation reduced microbiota-produced B vitamins. Supplementation with specific fibers restored these vitamins and modulated the immune system by altering local gut effector immune populations. The study highlights the role of dietary fibers in boosting microbiota-derived B vitamins and regulating immune function, emphasizing the importance of diet in maintaining immune health

Improving the growth and intestinal colonization of Escherichia coli Nissle 1917 by strengthening its oligopeptides importation ability

Sun and colleagues in Metabolic Engineering enhanced the growth and intestinal colonization of the probiotic Escherichia coli Nissle 1917 by improving its ability to import oligopeptides. Metabolomics studies identified limitations in amino acid uptake as a growth-limiting factor. By overexpressing a tripeptide-specific importer from Prevotella copri, they increased the bacterium's growth and colonization in the gut. This approach offers a strategy to improve the efficacy of probiotic treatments by enhancing nutrient acquisition capabilities

Microbiome and metabolome patterns after lung transplantation reflect underlying disease and

chronic lung allograft dysfunction

Martin and colleagues in Microbiome analyzed the microbiome and metabolome of bronchoalveolar lavage fluid from lung transplant recipients. They found that patterns in microbial communities and metabolite profiles correlated with the patients' underlying diseases and the development of chronic lung allograft dysfunction (CLAD). The study suggests that metabolomic and microbiome profiling could inform personalized management strategies for transplant patients and improve outcomes by monitoring and potentially modulating immune responses

Metabolomics in Neurological and Neurodegenerative Diseases

Metabolomics has provided valuable insights into neurological disorders by identifying metabolic alterations associated with disease states. These studies offer potential biomarkers for early diagnosis and uncover novel therapeutic targets. The following papers delve into the metabolomic changes in cerebrospinal fluid and serum, the discovery of new regulators of motor function, and the metabolic impacts of probiotics on neurodegenerative diseases

<u>Comprehensive analysis of the cerebrospinal fluid and serum metabolome in neurological diseases</u>

Otto and colleagues in the Journal of Neuroinflammation conducted an extensive metabolomic analysis of cerebrospinal fluid (CSF) and serum from patients with various neurological diseases, including Parkinson's disease and multiple sclerosis. Using nuclear magnetic resonance spectroscopy, they identified specific metabolite profiles that distinguished between disease groups. The study found that certain metabolites correlated with age and blood-brain barrier function, and that metabolome profiles could potentially aid in differentiating neurological diseases, contributing to improved diagnostic strategies

Ophthalmate is a new regulator of motor functions via CaSR: implications for movement disorders

Alhassen and colleagues in Brain discovered that the metabolite ophthalmate acts as a regulator of motor functions through the calcium-sensing receptor (CaSR). In mouse models of Parkinson's disease, they observed that ophthalmate levels surged following I-DOPA administration when dopamine synthesis was inhibited. Supplementing ophthalmate improved motor deficits, suggesting its potential as a therapeutic agent for movement disorders. This study highlights the role of metabolomics in identifying novel neuromodulators and therapeutic targets

Encapsulated Lactiplantibacillus plantarum improves Alzheimer's symptoms in APP/PS1 mice

Hu and colleagues in the Journal of Nanobiotechnology investigated the therapeutic effects of encapsulated Lactiplantibacillus plantarum on Alzheimer's disease (AD) symptoms in mice. The encapsulation protected the probiotics from gastrointestinal damage, leading to improvements in neuroinflammation, neuronal damage, and cognitive function. Metabolomics analyses showed that the treatment restored the balance of the intestinal microbiota and increased levels of beneficial metabolites. The study suggests that encapsulated probiotics could be a novel approach to ameliorate AD symptoms by modulating the gut-brain axis

Metabolomics in Cancer Metabolomics and Diagnosis

Metabolomics plays a crucial role in cancer research by uncovering metabolic alterations that contribute to tumor development and progression. These studies provide insights into potential biomarkers for early detection and targets for therapy. The following papers focus on metabolomic perturbations preceding prostate cancer diagnosis, metabolic heterogeneity in colorectal cancer., and phenotypic prediction of lymphoma

Perturbations in the blood metabolome up to a decade before prostate cancer diagnosis in 4387 matched case-control sets from the European Prospective Investigation into Cancer and Nutrition.

Grenville and colleagues in the International Journal of Cancer analyzed blood metabolites from participants up to ten years before prostate cancer diagnosis. They identified specific metabolites and metabolite patterns associated with an increased risk of developing prostate cancer. The study suggests that metabolomic profiling could serve as an early detection tool, improving risk stratification and potentially guiding preventive interventions.

Charting the metabolic biogeography of the colorectum in cancer: challenging the right-sided versus left-sided classification.

Jain and colleagues in Molecular Cancer investigated the metabolic profiles of colorectal cancer across different anatomical subsites. Using metabolomics, they found gradual changes in metabolite abundances from the cecum to the rectum and identified metabolites associated with patient survival. Their findings challenge the conventional classification of colorectal cancers into right-sided and left-sided, suggesting that metabolic profiling could lead to more precise classifications and personalized treatment strategies.

Metabolite, immunocyte phenotype, and lymphoma: a Mendelian randomization study.

Fan and colleagues in Frontiers in Immunology performed a Mendelian randomization study to explore the causal relationships between metabolites, immune cell phenotypes, and lymphoma risk. They identified bidirectional causal associations and found that certain immune cell phenotypes mediate the effects of metabolites on lymphoma development. The study enhances the understanding of lymphoma pathogenesis and highlights potential metabolic and immunological targets for intervention

Metabolomics in Metabolic Disorders and Aging

Metabolomics provides valuable insights into metabolic disorders and the aging process by identifying key metabolic pathways and potential biomarkers. These studies contribute to understanding disease mechanisms and developing targeted interventions. The following papers explore lysine metabolism in cold acclimation, inhibition of adipose triglyceride lipase in liver disease, and the prediction of diabetes progression using metabolomics

Cold exposure accelerates lysine catabolism to promote cold acclimation via remodeling hepatic histone crotonylation.

Xue and colleagues in Environment International studied the effects of cold exposure on lysine metabolism in humans and mice. They found that cold exposure accelerates lysine catabolism, leading to enhanced cold acclimation through changes in hepatic histone modifications. Lysine supplementation improved cold tolerance in mice, suggesting a potential therapeutic strategy for improving metabolic health in cold environments.

Inhibition of ATGL alleviates MASH via impaired PPARalpha signalling that favours hydrophilic bile acid composition in mice.

Dixon and colleagues in the Journal of Hepatology investigated the effects of inhibiting adipose triglyceride lipase (ATGL) on metabolic dysfunction-associated steatohepatitis (MASH). They found that ATGL inhibition improved liver health by altering bile acid composition and impairing PPARalpha signaling. The study provides insights into new therapeutic targets for MASH and underscores the importance of metabolomics in understanding liver diseases.

Nuclear magnetic resonance-based metabolomics with machine learning for predicting progression from prediabetes to diabetes.

Li and colleagues in eLife used nuclear magnetic resonance-based metabolomics combined with machine learning to predict the progression from prediabetes to diabetes. They identified a panel of nine metabolites that significantly improved risk prediction beyond traditional factors. The study demonstrates the potential of metabolomics in early detection and personalized intervention strategies for diabetes.

Methodological Advances in Metabolomics and Multi-Omics

Advancements in analytical methods enhance the capacity to conduct comprehensive metabolomics and multi-omics studies. These developments facilitate deeper insights into complex biological systems and disease mechanisms. The following papers highlight innovative techniques and resources that expand the capabilities of metabolomics research

The Addition of Transcriptomics to the Bead-Enabled Accelerated Monophasic Multi-Omics Method: A Step toward Universal Sample Preparation.

Breidenbach and colleagues in Analytical Chemistry introduced an improved method for multi-omics sample preparation, incorporating RNA extraction for transcriptomics analysis. This approach, known as the modified bead-enabled accelerated monophasic multi-omics (mBAMM) method, allows simultaneous analysis of proteomics, lipidomics, metabolomics, and transcriptomics from a single sample. The development represents a significant step toward universal sample preparation, enabling more comprehensive biological analyses.

Constructing HairDB to facilitate exposome research using human hair.

Chen and colleagues in Environment International developed HairDB, an online database compiling hair-related chemicals relevant to exposome research. By integrating data from metabolomics studies, literature, and existing databases, HairDB provides a comprehensive

resource for analyzing environmental exposures using human hair. This tool advances the field of exposomics by facilitating the identification of chemical exposures and their potential health impacts.

Archaeometabolomics characterizes phenotypic differences in human cortical bone at a molecular level relating to tobacco use.

Badillo-Sanchez and colleagues in Science Advances utilized archaeometabolomics to analyze cortical bone samples from historical human remains. They identified molecular differences in the bone metabolome associated with tobacco use, suggesting that metabolomic profiles can reveal lifestyle factors from archaeological specimens. The study demonstrates the potential of metabolomics in understanding historical human health and disease patterns, as well as the long-term effects of environmental exposures on bone metabolism.

Metabolomics in Agriculture and Food Sciences

Metabolomics is instrumental in agriculture and food science for optimizing crop quality, understanding plant metabolism, and improving nutritional content. The following papers explore how metabolomic analyses can guide harvest timing and enhance the functional properties of food products.

Integrated nutritional and functional components analyses reveal insights into the peel and pulp quality at different harvest times of 'Dahongpao' tangerine (Citrus reticulata Blanco)

Hu and colleagues in Food Chemistry analyzed the nutritional and functional components of 'Dahongpao' tangerine peel and pulp at different harvest stages. Using metabolomics, they found that the peel had the highest flavonoid content at the middle maturity stage, while polysaccharide content peaked at full maturity. The pulp also exhibited optimal nutritional properties at the middle stage. The study provides recommendations for optimal harvest times to maximize the nutritional and functional benefits of the tangerine

Cover crop root exudates impact soil microbiome functional trajectories in agricultural soils

Seitz and colleagues in Microbiome explored how root exudates from different cover crops affect soil microbiome functionality. Using metabolomics and metatranscriptomics, they found that distinct exudate profiles from four cover crop species led to unique microbial metabolic patterns over time. Specifically, exudates from sorghum and cereal rye enriched for novel microbial taxa and altered nitrogen cycling processes. The study emphasizes the potential of manipulating root exudate chemistry to target specific soil biogeochemical outcomes, enhancing agricultural productivity through biological precision practices

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Metabolomics Events

Bits & Bites # 09: Biochemical interpretation and

visualization of metabolomics data *New Course* November 7, 2024

Venue: Online

This course is taught by Prof. Oliver Fiehn, UC Davis. The level of the course is introductory, requiring no specific software or experience. In this short course, participants will focus on interpreting data, generating hypotheses, integrating biological and metabolomics data, and making the most of freely available online databases. The course provides practical tips on curation, data mapping, and visualization.

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

Check for more details

Alberta Metabolomics Day 2024

November 15, 2024

Venue: Edmonton, Canada

An event bringing together researchers, professionals, and students in the field of metabolomics. It is a one-day symposium offering a platform to explore the latest advancements, share innovative research, and foster collaborations through keynote presentations, poster sessions, and networking opportunities.

Check more about the symposium

Bits & Bites #10: Identification of unknown compounds in untargeted metabolomics using freely available software December 5, 2024

Venue: Online

This course is taught by Dr. Arpana Vaniya, UC Davis. The level of the course is introductory requiring basic knowledge of computer skills.

Short description of the course: Where do you start when a multitude of approaches exist to address the challenge of metabolite identification? There are so many options from mass spectral library searches, *in silico* fragmentation tools, and database searching. We will provide tips on

how to explore the landscape of compound identification, leverage *in silco* fragmentation tools, and gain valuable hands-on experience by using real-world challenges.

The tuition is \$350 per Bite and will take approx. 8 hours.

Check for more details

Imperial College London Metabolomics training course: Hands-on Data Analysis for Metabolic Profiling

December 9-13, 2024

Venue: Online

This 5 day course provides a comprehensive overview of data analysis for metabolic profiling studies focussing on data from NMR spectroscopy and Liquid Chromatography-Mass Spectrometry. It combines lectures and tutorial sessions using open-source software to ensure a thorough understanding of the theory and practical applications. To fully benefit from this course, attendees will ideally have a basic knowledge of analytic chemistry techniques.

The deadline for registering is November 29, 2024.

For more information and to register, click here.

Check for more details about the course

MANA SODAMeet

December 10, 2024

Venue: Online

The goal of SODA is to provide a community-driven resource of actively-maintained software, test datasets used for software benchmarking, and results produced by software. SODAMeets is a platform where data generators and computational scientists can share their use of software/data. During SODAMeets (every 2 months), two speakers will present on software or data they would like to share with the community, emphasizing how these software/data are used. Speakers will be requested to fill out a form on our SODA website so that we collect relevant information on these software/data presented.

GRC: Metabolomics and Human Health - The Interaction Between Humans, Lifestyles and the Environment Viewed through Metabolism

February 2 - 7, 2025

Venue: Ventura, California, USA

Metabolomics is the comprehensive study of the metabolome, the repertoire of metabolites present in cells, tissues, and body fluids. More recently, these metabolites are being implicated in the development of unhealthy ageing and diseases, positive and negative impacts of interaction with the exposome and the promotion of human health. The human metabolic profile is influenced by a number of factors including diet, genetics, environmental factors and the microbiome. Understanding the influence of these factors at a cellular and systemic level is key to deciphering the role of metabolites in human health and promotion of lifespan. In this Gordon Conference series, we highlight state of the art metabolomics technologies and how such technologies can be used to study human health. The conference will cover exciting new applications in the field such as epidemiology, cancer, nutrition, analytical chemistry and bioinformatics and translation to human benefit.

Check for more details

NIST SRM 1950 Beyond the Certificate of Analysis: mQACC Call to Provide Qualitative and Quantitative Data

Certified reference materials (CRM) values provide a known and standardized reference point against which the results of a metabolomic study can be compared. However, the certification of hundreds of individual metabolites is a cumbersome and time-consuming process. The Standard Reference Material (SRM) 1950, Metabolites in Frozen Human Plasma, is by far the most used reference material by the metabolomics community. NIST SRM 1950 provides certified and/or reference values for select metabolites and lipids such as fatty acids, electrolytes, vitamins, hormones, and amino acids. The metabolomics community would greatly benefit from consensus values and identification of metabolites and lipids in SRM 1950 that are not tied to a single analytical platform or method. This increases the accuracy, reliability, harmonization, and meaningful comparisons of metabolomic studies utilizing the material. Additionally, having more values and information available for SRM 1950 metabolites and lipids would allow researchers to

investigate a broader range of analytes in their studies, which in turn could lead to a better understanding of the underlying biology of the metabolic processes. To that end, the Reference and Test Materials Working Group of mQACC is actively collecting information on qualitative identifications and quantitative values of metabolites and lipids in NIST SRM 1950 beyond those listed on the NIST Certificate of Analysis. Any data from instrumental platforms with compound identification (LC-MS, GC-MS, NMR) are welcome to participate. The data was combined in order to produce a publicly available database of community-generated 1) consensus concentration values for quantified metabolites and lipids of critical interest within the community and 2) compounds identified but not quantified in SRM 1950.

More information and an example reporting form can be found at https://www.mqacc.org/srm1950

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Metabolomics Jobs

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Post Doctoral Fellow in Clinical Exposomics	Emory University	Atlanta, GA, United States	Emory University
Lab Scientist in		Basel, Basel-City	,

Metabolomics	Thermo Fisher Scientific	Switzerland	Roche
Application Scientist III	Thermo Fisher Scientific	Vilnius, Lithuania	Thermo Fisher Scientific
Data Scientist / Senior Data Scientist		Oxford, England	Metabolomics Society

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