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MetaboNews

This month in metabolomics

August, 2024
Vol 14, Issue 8

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

In This Issue

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

Members' Corner

Board of Directors

The Metabolomics Society Board of Directors is happy to welcome back (4) familiar faces to serve a second two-year term: Maria Eugenia Monge, Rick Dunn, Tomáš Pluskal and Lynn Vanhaecke!

We also welcome new faces to serve on the Board, congratulations to the new Directors:

- Nicholas Rattray, University of Strathclyde, UK
- Elizabeth Want, Imperial College London, UK
- Aurelia Williams, North-West University, South Africa

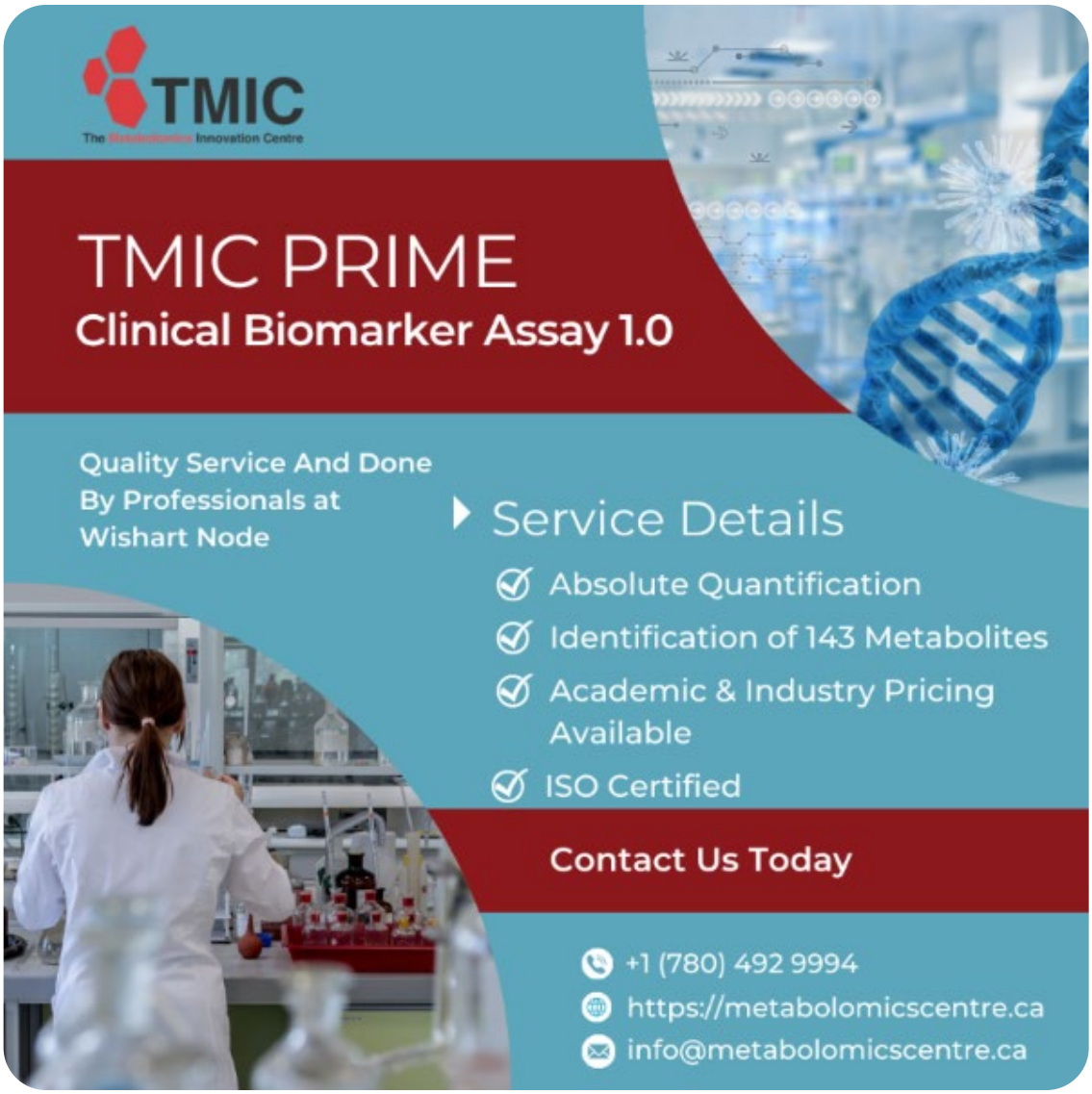
The term begins on October 1, 2024.

Next up: please vote in the upcoming Officer Election, as we have two important openings for the President and Secretary roles. Be on the lookout for a link to the poll in the next couple of weeks.

All the very best.

Roy Goodacre, University of Liverpool, UK

President, Metabolomics Society



The TMIC Prime service is an ISO accredited service which offers advanced metabolic profiling through a fully quantitative analysis of 143 metabolites using state-of-the-art mass spectrometry techniques. This service provides detailed insights into metabolic pathways, helping researchers and clinicians understand biochemical changes associated with diseases, drug responses, and nutritional interventions.

TMIC Prime supports a wide range of applications, including biomarker discovery and personalized medicine, by delivering precise and extensive metabolic data.

To learn more check out: https://metabolomicscentre.ca/service/tmic-prime/

International Affiliates' Corner

Réseau Français de Métabolomique et Fluxomique (RFMF)
Visit http://www.rfmf.fr/

Join the next RFMF Webinar on NMR Metabolomics on 12th September 2024
Don’t miss the upcoming RFMF webinar on **NMR Metabolomics** on 12th September 2024, from 3:00 PM to 4:30 PM (Paris time). The session, chaired by **Ghina HAJJAR** and **Audrey LE GOUELLEC**, will feature a keynote presentation by **Elizabeth ODAY,** CEO, CSO, and Founder of **Olaris, Inc.** (United States).

The event will also include presentations by:

- Gildas BERTHO (UMR8601 CNRS Université Paris Cité, France)
- Yan YAN (Imperial College London, United Kingdom)
- Marion MARAVAT (Plateforme MetaToul-MetaboHUB, France)

Join the webinar on exciting developments in NMR metabolomics here.

Polish Society of Metabolomics
Visit https://ptmet.pl/

The Polish Society of Metabolomics invites you to the annual 10th Conference of the Polish Society of Metabolomics - Metabolomics Circle.

This year, it will be a joint event of Metabolomics Circle (MetCircle2024) and Advances in Pharmaceutical Analysis (APA2024) Symposia.

It will take place on 15 -16 November in Lodz, Poland, at Lodz University of Technology. More details about the meeting are available here: https://metcircle-apa2024.org/

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Thailand Metabolomics Society (TMS)

Visit https://thailand-metabolomics.org/

Thailand Metabolomics Society
(TMS)

Please join us for the 2nd Thailand Metabolomics Society (TMS) Conference:

“Rise of Metabolomics in Thailand” to be held on October 3rd–4th, 2024, at the K Building, VISTEC, Rayong, Thailand.

Visit the website for details: https://conference.thailand-metabolomics.org/

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MetaboInterview

Dr. David Beale

Senior Research Scientist at CSIRO

Adjunct Associate Professor of RMIT University

Biography

Dr. David Beale is an experienced researcher with a demonstrated history of working in the research industry. Skilled in GC-MS and LC-MS based Metabolomics, Molecular Biology, Environmental Awareness, and Environmental Health. Dr. Beale is a strong research professional with a Doctor of Philosophy (PhD) focused in Analytical Chemistry from RMIT University.

How did you get involved in exposomics?

My journey into metabolomics began roughly 15 years ago, inspired by a year-end interdepartmental rapid-fire seminar series given by some friends while we were all completing our PhDs at RMIT University in Melbourne, Australia. One was studying inborn errors in metabolism in newborns, another was advancing the use of multidimensional gas chromatography for more accurate analysis of complex samples, and I was investigating innovative techniques for detecting pesticide contamination in water catchments. Following the seminar, we delved into a deep discussion about metabolomics, mass spectrometry, and their environmental applications over drinks at a local pub. Can we better link metabolomics with exposure-effects = exposomics. This conversation ignited my interest in exposomics and its potential to allow us to extend beyond simply measuring environmental contaminants, offering a fresh outlook on their effects on organisms and ecosystems beyond traditional markers such as mortality, morbidity, or reproduction. Around that time, I also commenced work at the Commonwealth Scientific and Industrial Research

Organisation (CSIRO), Australia's leading national research institution, where I engaged in various projects related to water quality and infrastructure reliability. Fortunately, CSIRO recognized the value of metabolomics and encouraged me to apply these approaches to diverse and innovative areas, including combating as pipe biofilms known to cause corrosion, drinking water network biofilms and anerobic wastewater treatment plants, among others.

In 2014, after relocating to Brisbane with CSIRO, I began focusing exclusively on environmental metabolomics and started developing the idea of omics-based ecosurveillance (conceptually outlined in Figure 1). This direction was shaped by discussions around an environmental metabolomics book project we were working on at the time, "Applied environmental Metabolomics: Community insights and guidance from the field." Our focus for omics-based tools is not to replace current environmental monitoring approaches but add another line of evidence to inform the function, health, fitness, and resilience of studied taxon. Currently, I lead a team that uses omics tools coupled with traditional methods to monitor environmental changes caused by both abiotic and biotic stress factors. Our team is particularly interested in how industrial pollutants affect wildlife and ecosystem function, and how they can address gaps in existing regulatory frameworks.

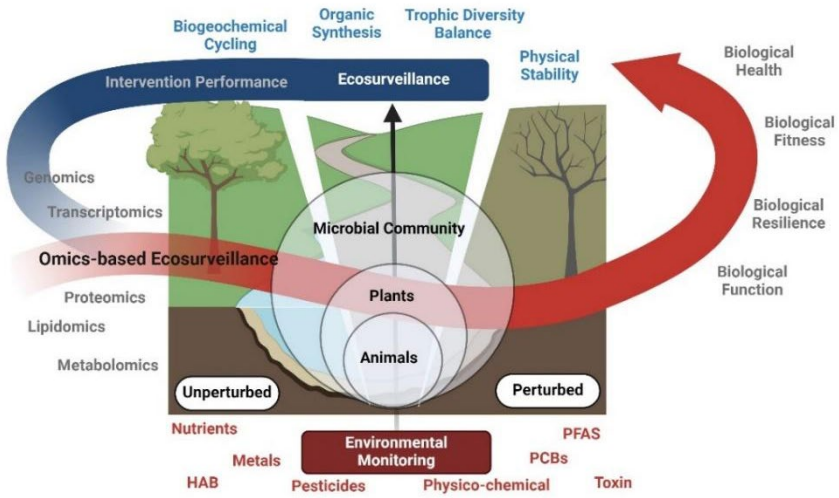

Figure 1. An overview of an ecosurveillance framework that encompasses omics-based technologies within a monitoring and surveillance setting.

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

With our recent focus on researching a range of contaminants impacting Australian wildlife, the most exciting aspect of our exposomics/environmental metabolomics work now is the field sampling. We have multiple ongoing projects that involve sampling and collecting wildlife specimens from native frogs, freshwater turtles, marine turtles, crocodiles, dugongs, seagrass, sea birds, and penguins (I am sure there are more, but that's the list of

animals we are actively working on currently). We also have been researching estuarine sediments over the last decade within pristine and industrial settings, focusing on understanding microbial member composition and measured functions using 16S sequencing techniques and metabolomics. Being able to explore different landscapes and ecosystems, interacting with vastly different wildlife, and undertaking impactful research – it is all very exciting!

We recently completed a major project in collaboration with the Queensland Environmental Regulator. We collected samples from several freshwater sites across Queensland, which have a well-documented PFAS profile. We then measured the PFAS levels that accumulated in the turtles and investigated the impact using omics-based tools (proteomics, lipidomics, and metabolomics). Working with these beautiful animals was a definite highlight, and knowing the research outputs are significantly impacting how we view PFAS levels in the environment. In fact, the research we did with the Environmental Regulator was discussed during Qld parliament's 'Health, Environment and Agriculture Senate Committee' meeting. The Parliament Committee discussion included topics on QLDs new PFAS compost limits and its regulation of the compost industry, the turtle work was undertaken downstream of a large composting area, and demonstrated the impacts unregulated industry can have to the environment. Observing the application of these tools in a regulatory setting and seeing their contribution to the development of adverse outcome pathways that have an influential role with state government was quite fulfilling.

Papers that are a direct result of our freshwater turtle - PFAS research with the Queensland Environmental Regulator include**:**

- Partitioning of PFAS to serum, tissues, eggs, and hatchlings of an Australian freshwater turtle (sciencedirectassets.com)
- Metabolic disruptions and impaired reproductive fitness in wild-caught freshwater turtles (Emydura macquarii macquarii) exposed to elevated per and polyfluoroalkyl substances (PFAS)
- Bioaccumulation and impact of maternal PFAS offloading on egg biochemistry from wild-caught freshwater turtles (Emydura macquarii macquarii)
- Bioaccumulation and metabolic response of PFAS mixtures in wild-caught freshwater turtles (Emydura macquarii macquarii) using omics-based ecosurveillance techniques
- Perturbation of the gut microbiome in wild-caught freshwater turtles (Emydura macquarii macquarii) exposed to elevated PFAS levels
- Host -Gut Microbiome Metabolic Interactions in PFAS-Impacted Freshwater Turtles (Emydura macquarii macquarii)

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

At the CSIRO, several initiatives have exposomics and environmental metabolomics at the forefront – for example, there is an extensive PFAS research program that is working to enhance environmental monitoring programs and provide the much-needed effects-based evidence that is being driven by our Ecosurevillance Systems Team and described briefly above. This includes measuring both emerging (i.e., PFAS) and legacy (i.e., heavy metal) contaminants, using targeted and non-targeted approaches, coupled with an omics-based effects assessment in non-model wildlife taxa (i.e., crocodiles, dugongs, turtles and other wildlife). This typically involves a range of omics-based resources and approaches being used, from generating new genome resources via our Applied Genomics Initiative, through to analyzing the proteome, lipidome and metabolome of various animal tissues and fluids.

We have complementary initiatives that build upon our research monitoring the effects of contaminants, such as our research investigating designer microbes for bioremediation of PFAS and bioelectrochemical stimulation for the degrading of PFAS on the environment. For example, the gut microbiome from the freshwater turtles exposed to PFAS that we sampled has been sequenced and several microbial targets isolated and evaluated as part of the designer microbes for bioremediation portfolio. We also have a portfolio of research investigating the use of insects as engineers for tackling difficult wastes – such as using wax moth larvae that are known to invade bee hives and eat their wax. We use these omics-based ecosurveillance tools to see how these invasive pests and other insects handle a non-traditional plastic diet.

We are collaborating with several research institutes and universities locally, such as Australian Institute of Marine Sciences (AIMS) and the University of Sydney to investigate the metabolome and chemical cues released by invasive crown of thorn starfish that damage coral reefs across the Great Barrier Reef; researchers at the University of Queensland investigating ecological threats to crocodiles; Indigenous ranger groups concern about climate change impacts to nesting marine turtles; PhD students at La Trobe University, University of Queensland and Griffith University looking at a range of wildlife exposome-based projects.

What is happening in your country in terms of Exposomics?

There's considerable activity in the field – numerous research teams across Australia are engaged in environmental metabolomics and conducting exposomics-related research, whether through observational studies or controlled exposure experiments. We're all linked or at least informed about each other’s projects through organizations like the Australian and New Zealand Metabolomics Society or the Australian Society of Environmental

toxicology and Chemistry (SETAC), along with their meetings and events.

I also serve as a co-chair for the international SETAC omics interest group, which provides me with a wider view of the global developments in this field. I have enjoyed short term placements with leading researchers and labs specializing in environmental metabolomics and other omics-based ecotoxicology research, including those at the US EPA, the Canadian Department of Environment and Climate Change, and notable academic institutions (i.e., Lawrence Berkeley National Laboratory, TMIC at University Alberta, University of Florida). During these placements, it's been acknowledged that Australia is at the forefront of environmental metabolomics. This coming autumn, I plan to undertake a three-month placement with some global leaders within Europe and the UK.

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

We are currently working closely with several state-based Environmental Regulators, and they are interested in using these omics-based ecosurveillance tools as part of their investigations into contamination events or compliment ongoing monitoring programs. We don’t see these new omics-based regulatory tools being used in isolation, instead we see them combined with current methods to provide an additional line of evidence. What we are aiming towards is a future where we have a large robust dataset of omics data tied to well characterized environmental datasets, wildlife, model and non-model organisms, and contamination concentration data that then facilitates a general practitioner approach to environmental health – akin to us going to our GP and getting a blood test for assessing current health and projected health trajectory. We see omics-based ecosurveillance approaches using multiple levels of omics-based data that will bring a greater understanding of the natural and perturbed environment.

As you see it, what are Exposomics' greatest strengths?

In simple terms, it serves as an additional line of evidence for risk assessment. While our capabilities in detecting environmental contaminants are advanced with several established and standardized techniques and methods now routinely available, gauging the consequence of those contaminants remains challenging, especially when effects are not immediately apparent or obvious, such as death or illness. By applying metabolomics with an exposomics lens, along with broader omics approaches, allows us a deeper understanding of the biological impact that follow exposure to these contaminants, which is often at sub-lethal and trace concentrations, something most conventional methods fail to reveal. However, this powerful and deep insight comes with a level of complexity that may be unfamiliar to many end users, such as Regulators and Government agencies.

What do you see as the greatest barriers for Exposomics?

In Australia, the primary obstacle is the insufficient usage and widespread adoption of these environmental metabolomics tools and techniques beyond academia into regulatory investigations and governmental initiatives. Regulators recognize the value of environmental metabolomics and exosome methods, but they are delayed in integrating them into government strategies. This might be partly due to the restricted public access to data from established contaminant studies or exposome observational research when they are conducted under regulatory stipulations. The lack of standardization in methods across the metabolomics community also hampers broader acceptance, along with limited availability to end users of the necessary expertise, equipment, and analytic resources for data (or the associated high costs to access it externally).

What improvements, technological or otherwise, need to take place for Exposomics

to really take off?

It feels like we now have critical mass in genomic resources, analytical technologies, and bioinformatics resources available within CSIRO. These facilities and resources have provided unprecedented insights into the composition, structure, function, and control of the genome, transcriptome, proteome, and metabolome in non-model and exotic Australian wildlife, shedding light upon known and unknown biological pathways and phenotypes. Making these technologies more accessible will also help to address remaining challenges in climate change and ecological and exposure risks. For the application of metabolomics to ecological/environmental monitoring, the primary issues such as sample and genetic heterogeneity, and limited genomic resources for non-model species complicate data interpretation and limit the potential for integration with other 'omes' to obtain systems-level information. Improvement of sampling techniques such as 'single-pot' sample extractions of valuable and often limited wildlife tissues could be useful in ensuring the use of a single sample (tube) for multiple omic measurements for a more resolved data interpretation. Additionally, de novo genome sequencing and species-specific database construction via advanced genomics annotation pipelines (CSIROs Applied Genomics Initiative) would be valuable to identify and validate markers for monitoring purposes. The consideration of intra- and inter-species population diversity, genetic polymorphism, phenotypic plasticity, and developmental stages (including the alternative splicing, polypeptide cleavage, post-translational modification) should also inform metabolome to proteome measurements (and other 'omics-based outputs) to better understand taxonomically similar species on a system level.

Another area that will advance the uptake of environmental metabolomics and exposomics is the improvement of metabolite identification. At present, many of what is labelled as 'features' in metabolomics datasets have not been identified. This limits our potential gain in knowledge and understanding of environmental processes, pollution impacts or key biological processes in non-model systems. However, a short-term solution is to collect robust environmental metadata around these unidentified features while annotation pipelines are further developed. This could allow them to be correlated and characterised in an environmental context, even if we don't know their specific function (e.g. metabolite feature X always occurs within Y environments with high metal loads, etc.). At this point, two main strategies for dealing with metabolomics datasets (which tend to be very large) have involved (1) the establishment of spectral databases to aid with individual feature identification, e.g. the Human Metabolome Database (www.hmdb.ca) and METLIN (https://metlin.scripps.edu/), and (2) developing workflows and analytical packages to facilitate multivariate statistics and multi-layer data integration on individual experimental outcomes. The creation of interactive and open-access databases of pollutants such as the toxic exposome database (http://www.t3db.ca), DrugBank (https://go.drugbank.com), and the EPA's non-targeted analysis (NTA) database have helped, but each lists data on

contaminants/toxicants, not the metabolic response(s) to such compounds. What would help in the future is a library of metabolite profiles for model species exposed to specific pollutants or mixtures of pollutants as a dedicated tool to facilitate environmental monitoring in complex aquatic environments. The knowledge and infrastructure from existing metabolomics databases could be used for data management, interactive storage, and access to such a system, but it would be reliant on high-quality data from the community to function. Such a database that is publicly available and easily searchable would facilitate the use of metabolomics in environmental science by allowing scientists to compare the results of the analysis of a system, to the metabolic response(s) of the organisms to known pollutants/toxicants (further building upon the 'Web of microbes' exometabolomics database for linking chemistry and microbes, as an example).

How does the future look in terms of funding for Exposomics?

The future looks bright in terms of funding! Numerous funding opportunities exist to advance research in environmental metabolomics and exposomics, usually aligned with the strategic objectives established by government funding agencies, as well as industry and environmental interest groups. The integration of omics technologies in these grants and calls for proposals is becoming more frequent among applicants, and the research community often emphasizes the importance of going beyond short-term funding periods to conduct studies across broader geographic areas and over longer timeframes. I see this trend more in the proposals I am being asked to review.

Of course, the funding outlook can always improve. One challenge is overcoming the perception that environmental metabolomics or exposomics studies lack novelty and feed into a larger program of routine monitoring or 'stamp collecting' of different data. Yet, within a regulatory setting, this is needed to incite a change from business-as-usual approaches to new omics-based approach methods. As an example, for omics-based studies to be conducted in parallel with current environmental monitoring approaches that demonstrate their value-add to the status-quo, regulators and funding models need to account for the perceived inherent risk of trialling these new approaches (and allow for financial mechanisms to include additional analytical costs and help to 'carry' the regulatory risk of just using an omics-only approach – they cannot stop ongoing monitoring programs in lieu of omics-based methods). Furthermore, funding agencies need to allow for open-ended studies that include (or rely on) nontargeted data but also encompass repeat non-target/omics measures over time (i.e. monthly and yearly) that can seem very open-ended to a regulator. Only then omics-guided ecosurveillance and exposomics can improve management intervention opportunities, decision making, and policies, but there are currently limited practical examples of these tools guiding these processes.

What role can Exposomics standards play?

Standards are crucial, especially for integrating these tools into routine monitoring and pollution investigations by regulators. Adopting standards for environmental metabolomics and exposomics will be essential to move these methods from academic research to practical use by regulators and commercial laboratories offering them as services.

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

There are so many cool projects focusing on environmental metabolomics and exposomics that are happening right now, not just here in Australia but all over the globe. It's exciting to think about the progress and advancements that are on the horizon and how it's going to benefit us as a society, our surrounding environment and all the inhabiting animals and plants we affect.

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MetaboReads

This month's articles explore some of the latest advancements in metabolomics research, highlighting diverse applications across microbial pathogenesis, environmental health, cardiovascular disease, therapeutic innovation, precision medicine, and industrial biotechnology. Metabolomics continues to show its promise as a critical enabling tool across multiple research disciplines and industries, revealing the broad impact of this powerful approach on our understanding of biological systems.

Microbial Metabolism and Host Interactions

Microbial metabolism and its interaction with the host environment play a crucial role in determining the outcome of infections and chronic diseases. The studies in this section explore how pathogens manipulate host metabolic pathways to establish infection, sustain their survival, and outcompete other microbial species.

A Metabolomics Pipeline Highlights Microbial Metabolism in Bloodstream Infections

Mayers et al. in CELL introduced a comparative metabolomics pipeline designed to unravel microbial metabolic features within a host environment, focusing on gram-negative bloodstream infections (BSI). The study identified elevated levels of bacterially derived acetylated polyamines during BSI, driven by the enzyme SpeG. Inhibiting SpeG not only reduced bacterial proliferation but also increased membrane permeability, enhancing the efficacy of antibiotics against resistant strains. This approach highlights the potential of targeting pathogen-specific metabolic pathways to combat antimicrobial resistance (AMR).

Staphylococcus Aureus Adapts to Exploit Collagen-Derived Proline During Chronic Infection

Urso et al. in Nature Microbiology examined how Staphylococcus aureus adapts to the host environment during chronic infections. The study revealed that S. aureus upregulates collagenase during chronic infection, enabling the bacterium to degrade host collagen and utilize proline to fuel its tricarboxylic acid (TCA) cycle. This metabolic adaptation allows S. aureus to outcompete non-adapted strains, suggesting that targeting collagen degradation and proline metabolism could be a viable strategy to combat chronic S. aureus infections.

Environmental Exposures and Health

The studies in this section explore the complex relationship between environmental exposures and health, particularly focusing on how external toxicants and pollutants can disrupt biological systems. Through advanced metabolomics and multi-omics approaches, these studies uncover

the molecular mechanisms by which environmental factors, such as toxic gases and industrial chemicals, impact organismal health, offering insights into potential mitigation strategies.

Mucosal Organs Exhibit Distinct Response Signatures to Hydrogen Sulphide in Atlantic Salmon (*Salmo Salar*)

Ara-Diaz et al. in Ecotoxicology and Environmental Safety studied the impact of hydrogen sulfide (H2S) exposure on the mucosal defenses of Atlantic salmon. The research revealed that while skin mucosa was relatively resilient, the gills and olfactory rosette were highly sensitive to H2S, exhibiting strong inflammatory responses. Despite the presence of detoxification pathways, the study found that prolonged exposure to sub-lethal levels of H2S triggered stress-related gene expression. Metabolomic analysis of skin and gill mucus identified alterations in amino acid biosynthesis and metabolism, underscoring the importance of assessing environmental toxicants' impact on aquatic life.

Multi-Omics Analysis and the Remedial Effects of Swertiamarin on Hepatic Injuries Caused by CCl_4

Li et al. in Ecotoxicology and Environmental Safety conducted a comprehensive multi-omics analysis to elucidate the protective effects of Swertiamarin on liver injury induced by CCl4 in mice. The study found that Swertiamarin treatment mitigated liver damage by reducing oxidative stress, inflammation, and fibrosis. Metabolomic profiling revealed that Swertiamarin modulates antioxidant enzymes and pathways involved in lipid metabolism, offering a potential therapeutic approach for treating environmental toxin-induced liver injuries.

Metabolic Dysregulation in Cardiovascular Diseases

Cardiovascular diseases are often accompanied by profound metabolic disturbances that contribute to disease progression and poor clinical outcomes. The research in this section investigates the metabolic signatures associated with heart failure, aiming to identify biomarkers and metabolic pathways that could be targeted for improved diagnosis and therapy.

Plasma Myo-Inositol Elevation in Heart Failure: Clinical Implications and Prognostic Significance. Results from the **BE**lgian and **CA**nadian **ME**tabolomics in **HF**pEF (BECAME-HF) Research Project

Poupleur et al. in EBioMedicine explored the role of myo-inositol in heart failure with preserved ejection fraction (HFpEF). Using mass spectrometry, the study measured plasma myo-inositol levels in patients with heart failure and found that elevated levels were particularly pronounced in HFpEF patients. Myo-inositol was associated with worse clinical outcomes and correlated with markers of cardiac fibrosis and kidney dysfunction. This suggests that targeting myo-inositol transport and metabolism could be a novel approach for managing HFpEF.

Landscape of Glycolytic Metabolites and Their Regulating Proteins in Myocardium from Human Heart Failure with Preserved Ejection Fraction

Koleini et al. in European Journal of Heart Failure investigated glycolytic metabolism in the myocardium of HFpEF patients, using both targeted and non-targeted metabolomics. The study identified significant reductions in key glycolytic intermediates such as glucose-6-phosphate and

fructose-1,6-biphosphate, along with decreased expression of their corresponding enzymes. This metabolic profile persisted even after adjusting for common comorbidities like obesity and diabetes, highlighting the intrinsic metabolic inflexibility in HFpEF myocardium.

Therapeutic Metabolomics and Novel Treatment Strategies

Metabolomics is increasingly being leveraged to develop innovative therapeutic strategies for a range of metabolic diseases, including cancer and hyperuricemia. The studies in this section showcase how manipulating metabolic pathways, whether through targeting specific enzymes or utilizing novel drug delivery systems, can lead to significant advancements in treatment efficacy and patient outcomes.

Progesterone Boosts Abiraterone-Driven Target and NK Cell Therapies Against Glioblastoma

Chen et al. in Journal of Experimental & Clinical Cancer Research explored a novel therapeutic strategy for glioblastoma (GBM) by combining progesterone with abiraterone. The combination therapy significantly enhanced apoptosis in TMZ-resistant GBM cells and improved survival in mouse models. Metabolomics analysis revealed that the therapy suppressed mitochondrial respiration and glycolysis in GBM cells, while also boosting NK cell-mediated immunity. These findings suggest that this combination could be a promising treatment approach for GBM.

Atavistic Strategy for the Treatment of Hyperuricemia via Ionizable Liposomal mRNA

Zhang et al. in Nature Communications proposed an atavistic strategy to treat hyperuricemia using ionizable liposomal mRNA (mUox) that encodes urate oxidase (Uox), an enzyme that humans lost during evolution. The study demonstrated that a single dose of mUox paired with an ionizable lipid nanoparticle significantly reduced serum uric acid levels in murine models for several weeks, as confirmed by metabolomics analysis. This innovative approach shows promise for long-term management of hyperuricemia and associated conditions like gout and cardiovascular disease.

Effective Prevention and Treatment of Acute Leukemias in Mice by Activation of Thermogenic Adipose Tissues

Chen et al. in Advanced Science reported that activating thermogenic adipose tissues (TATs) in mice via cold exposure or beta-3 adrenergic receptor agonists significantly suppressed the progression of acute myeloid leukemia (AML) and acute lymphoblastic leukemia (ALL). The study showed that TAT activation impaired glycolytic metabolism in leukemic cells, reducing their growth and invasiveness. Additionally, combining TAT activation with chemotherapy enhanced anti-leukemic effects while reducing chemotoxicity, offering a new therapeutic paradigm for hematological malignancies.

Metabolomics in Precision Medicine and Personalized Health

The shift towards precision medicine, tailoring treatments to individual patients based on their specific metabolic profiles, continues to be supported by the latest advances in metabolomics. The research in this section highlights the use of metabolomics to predict disease risk, monitor therapeutic responses, and personalize medical interventions, particularly in the context of chronic

and complex diseases.

Personalized Metabolic Whole-Body Models for Newborns and Infants Predict Growth and Biomarkers of Inherited Metabolic Diseases

Zaunseder et al. in Cell Metabolism developed personalized whole-body metabolic models (WBMs) for newborns and infants, spanning the first 180 days of life. These models, parameterized with organ-specific dynamics and nutritional data, accurately predicted growth and changes in biomarkers related to inherited metabolic diseases. The infant-WBMs hold promise for creating digital metabolic twins, which could revolutionize pediatric care by enabling personalized monitoring and treatment of metabolic disorders.

Age-Related Patterns of Microbial Dysbiosis in Multiplex Inflammatory Bowel Disease Families

Jacobs et al. in Gut investigated age-related patterns of microbial dysbiosis in families with a high risk of inflammatory bowel disease (IBD). Using 16S rRNA gene sequencing and global untargeted metabolomics, the study found that dysbiosis progresses from infancy through adulthood in unaffected relatives. The research identified specific faecal and serum metabolites associated with dysbiosis, suggesting these could serve as biomarkers for early IBD risk prediction and management.

Early and Long-Term Responses of Intestinal Microbiota and Metabolites to ^{131}I Treatment in Differentiated Thyroid Cancer Patients

Lu et al. in BMC Medicine examined the effects of 131I therapy on gut microbiota and metabolism in patients with differentiated thyroid cancer. The study found that multiple high doses of 131I disrupted gut microbiota balance and altered metabolic pathways, such as linoleic acid and tryptophan metabolism. These findings underscore the importance of monitoring gut microecology during cancer treatment to minimize radiotoxicity and optimize therapeutic outcomes.

Metabolomics in Food Science and Agricultural Biotechnology

Food science and agricultural biotechnology are rapidly evolving fields where metabolomics is playing an expanding role in enhancing safety, quality, and sustainability. The studies in this section explore how metabolomic approaches can be applied to improve food packaging, understand microbial dynamics in agriculture, and develop crops with enhanced stress tolerance, thereby addressing global challenges in food security and environmental sustainability.

Cinnamon Essential Oil Induced Microbial Stress Metabolome Indicates its Active Food Packaging Efficiency when Incorporated into Poly Vinyl Alcohol, Engineered with Zinc Oxide Nanoparticles and Nanocellulose

Jose et al. in International Journal of Biological Macromolecules investigated the antimicrobial properties of nanocomposite films containing cinnamon essential oil, zinc oxide nanoparticles, and nanocellulose. The study used metabolomics to analyze the microbial stress response, demonstrating that these films effectively inhibited the growth of common foodborne pathogens. This research could lead to the development of safer, more sustainable food packaging materials.

Nutrient and Moisture Limitations Reveal Keystone Metabolites Linking Rhizosphere

Metabolomes and Microbiomes

Baker et al. in Proceedings of the National Academy of Sciences of the United States of America identified keystone metabolites in the rhizosphere of switchgrass under nutrient and moisture stress, linking these metabolites to microbial community dynamics. The study found that serotonin and ectoine, which were enriched under nitrogen-replete conditions, played key roles in shaping root architecture and microbial growth. These findings have broader implications for understanding how plant-microbe interactions could influence agricultural productivity through metabolic reprogramming.

Unraveling the Spoilage Characteristics of Refrigerated Pork using High-Throughput Sequencing Coupled with UHPLC-MS/MS-Based Non-Targeted Metabolomics

Yi et al. in Food Chemistry employed high-throughput sequencing and UHPLC-MS/MS-based non-targeted metabolomics to explore pork spoilage. The study identified core microbiota, such as Pseudomonas and Serratia, that contribute to spoilage by producing biogenic amines and other metabolites. The findings suggest that monitoring specific metabolites could serve as biomarkers for early detection of spoilage, improving food safety.

Passion Fruit HD-ZIP Genes: Characterization, Expression Variance, and Overexpression *PeHB31* Enhanced Drought Tolerance via Lignin Pathway

Ma et al. in International Journal of Biological Macromolecules characterized HD-ZIP genes in passion fruit, focusing on PeHB31, which was found to enhance drought tolerance via lignin pathway modulation. Metabolomics revealed that overexpression of PeHB31 increased lignin content in transgenic Arabidopsis plants, improving their drought resistance. This study provides a foundation for developing crops with enhanced stress tolerance, which is crucial for agricultural sustainability in the face of climate change.

Industrial Biotechnology and Environmental Applications

Industrial biotechnology harnesses biological systems to produce valuable products and address environmental challenges. The research in this section focuses on the application of metabolomics in industrial processes, from optimizing microalgae-based wastewater treatment to engineering plants for the production of bioactive compounds. These studies underscore the potential of metabolomics to drive innovation in sustainable industrial practices.

Removal Mechanisms and Metabolic Responses of C*hlorella Pyrenoidosa* to Dissolved Organic Phosphorus

Wu et al. in Bioresource Technology investigated the metabolic responses of Chlorella pyrenoidosa to different dissolved organic phosphorus (DOP) forms, including ATP, glucose-6-phosphate, and beta-glycerophosphate. The study found that the uptake of DOP followed pseudo second-order kinetics and that different DOP sources significantly influenced the central carbon metabolism of the algae. The findings provide valuable insights into optimizing microalgae-based biotechnologies for wastewater treatment.

Steroidal Scaffold Decorations in *Solanum* Alkaloid Biosynthesis

Lucier et al. in Molecular Plant focused on the biosynthesis of steroidal glycoalkaloids (SGAs) in Solanum species. By combining metabolomics with transcriptomics, the researchers identified enzymes responsible for converting cholesterol into bioactive SGAs, such as alpha-solasonine and alpha-solamargine. These SGAs have documented anti-cancer and anti-inflammatory properties, and the study provides a toolkit for engineering these molecules in alternative hosts using synthetic biology.

The Metabolomist Podcast

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Metabolomics Events

Bits & Bites # 06: Using the GNPS for Metabolomics Data Analysis and Visualizations

September 12, 2024

Venue: Online

This course is taught by Prof. Mingxun Wang, UC Riverside. The level of the course intermediate, requiring no GNPS account but no specific software or prior programming experience. In this short course, participants will get familiar with GNPS (Global Natural Products Social Molecular Networking) a web-based mass spectrometry ecosystem, and learn how to look at your data using classical molecular networking. Explore GNPS Tools for MassIVE data navigation, including classical molecular networking, data selection, mastering molecular network workflows, interactive LC/MS visualization, and compound identification. Uncover insights into intricate mass spectrometry data efficiently. Exciting material to be covered with new additions to GNPS, that will be launched in the Wang Lab in 2024.

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

Check for more details

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Bits & Bites # 07: Using MetaboAnalyst for Metabolomics Statistics and Data Visualizations

October 3, 2024

Venue: Online

This course is taught by Prof. Jeff Xia, McGill University. The level of the course is introductory, requiring basic computer skills and no prior programming experience is necessary. In this short course, participants will focus on mastering MetaboAnalyst 5.0, the robust platform for statistical analysis in metabolomics. Learn data input, preprocessing, and key analyses like PCA, PLS-DA, and OPLS-DA. Explore functional analysis techniques, and biomarker identification, and tackle complex metadata for robust statistical insights in metabolomics data.

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

Check for more details

Metabolomics in Toxicology course

October 7 – 9, 2024

Venue: School of Biosciences - University of Birmingham, England

This 3-day course introduces the use of LC-MS based metabolomics to study toxicological processes and toxicological risk. This course provides hands-on experience for both the Q Exactive™ Plus (QE+) and Orbitrap ID-X™ Tribrid™ mass spectrometers, using a single toxicological case-study to guide delegates through an introduction to metabolomics in toxicology, from experimental design to metabolite identification.

This course is led and delivered by five experts in the field of metabolomics and includes lectures, laboratory sessions, and computer workshops to provide a detailed overview of how metabolomics can be used in toxicological research.

Early-bird registration deadline: **September 7, 2024 (terms and availability apply)**.
For more information, including registration, click here.

Learn more here

MANA SODAMeet

October 8, 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.

Join the web seminar

Untargeted Metabolomics LC/MS Data Processing course

October 14 – 16, 2024

Venue: School of Biosciences - University of Birmingham, England

This 3-day course is designed to address challenges associated with untargeted metabolomics data processing, and is recommended for either (i) individuals who have already completed an introductory-level BMTC course, or (ii) delegates with existing intermediate experience operating LC-MS metabolomics, and will provide trainees with furthered skills in metabolomics data processing and analytics.

Delegates will be provided with real LC-MS datasets for hands-on analysis, and throughout several sessions will be guided through various tools for metabolomic data processing and statistical analysis, including XCMS, univariate statistics, multivariate analysis, and annotation processing.

Early-bird registration deadline: **September 7, 2024 (terms and availability apply)**.
For more information, including registration, click here.

Learn more here

6th Annual Metabolomics MANA Conference

October 21 – 24th, 2024

Venue: Tampa, Florida

The 6th Annual MANA Conference, hosted by Drs. Tim Garrett and John Koomen, will take place from October 21-24, 2024, in Tampa, Florida. This year's conference features an impressive lineup of plenary speakers, including Drs. Tao Huan, Oliver Fiehn, Gina DeNicola, Patricia Scaraffia, and Julia Laskin, who will present their cutting-edge work in metabolomics.

Poster abstract submission deadline: **closed on August 16, 2024**
Early-bird registration deadline: **August 30th, 2024**
For more information, including registration, click here.

Learn more here

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Bits & Bites # 08: Statistics in R for Metabolomics *New Course*

October 24, 2024

Venue: Online

This course is taught by Dr. Christopher Brydges from SomaLogic. The level of the course is intermediate, requiring basic knowledge of statistics, such as understanding what a t-test is and when to use one. In this short course, participants will focus on analyzing case/control study data and crafting compelling data visualizations in R. Explore R's core concepts, master data loading, and manipulation including missing data imputation. Learn essential data analysis techniques like univariate vs. multivariate approaches and delve into creating and customizing impactful graphs and plots.

Required Software: R and RStudio (Exact versions to be specified nearer the course date)

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

Check for more details

2025 Metabolomics and Human Health

February 2 - 7, 2025

Venue: Ventura, California

The Metabolomics and Human Health GRC is a premier, international scientific conference focused on advancing the frontiers of science through the presentation of cutting-edge and unpublished research, prioritizing time for discussion after each talk and fostering informal interactions among scientists of all career stages. The conference program includes a diverse range of speakers and discussion leaders from institutions and organizations worldwide, concentrating on the latest developments in the field. The conference is five days long and held in a remote location to increase the sense of camaraderie and create scientific communities, with lasting collaborations and friendships. In addition to premier talks, the conference has designated time for poster sessions from individuals of all career stages, and afternoon free time and communal meals allow for informal networking opportunities with leaders in the field.

Applications for this meeting must be submitted by **January 5, 2025**. Please apply early, as some meetings become oversubscribed (full) before this deadline.

GRC Education Requirements: Undergraduates or those who have not obtained a bachelor's degree in science/engineering (or acceptable equivalent) are not eligible to apply to attend Gordon Research Conferences or Seminars.

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

Metabolomics Jobs

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Metabolomics Jobs

If you have a job to post, please email the MetaboNews team at metabolomics.innovation@gmail.com

We may remove a listing after 6 months if we do not receive a confirmation that it is still necessary. However, if you would like us to repost it, please contact us.

Job Title	Employer	Location	Source
Scientific Associate LC-MS proteomics and metabolomics	Idorsia Pharmaceuticals Ltd	Basel, Switzerland	Idorsia Pharmaceuticals Ltd
Research Associate (Fixed term)	University of Cambridge	Cambridge, UK	University of Cambridge
Postdoctoral Research Associate I, Equine Genetics and Genomics	University of Arizona	Tucson, AZ, USA	University of Arizona
Lab Scientist in Metabolomics	Thermo Fisher Scientific	Basel, Basel-City, Switzerland	Roche
Application Scientist III	Thermo Fisher Scientific	Vilnius, Lithuania	Thermo Fisher Scientific
12 PhD positions in Xpose doctoral training unit (various topics)	Luxembourg Institute of Health (LIH), University of Luxembourg, Luxembourg Institute of Socio-Economic Research (LISER)	Luxembourg City or Belval, Luxembourg	Xpose, Luxembourg Institute of Health (LIH)
Data Scientist / Senior Data Scientist		Oxford, England	Metabolomics Society
Research Associate	MetaCom, Institute for Plant Biochemistry	Halle, GE, Germany	Leibniz Institute of Plant Biochemistry
Post-Doc Fellowship in Cancer Epidemiology	American Cancer Society	Atlanta, GA, USA	American Cancer Society

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MetaboNews Feedback Form

Thank you for being a part of MetaboNews! Your input means a lot to us, and we're eager to hear your thoughts on how we can improve our newsletter. We've put together a brief, anonymous survey with just two mandatory questions that won't take more than a minute of your time. Your feedback is invaluable, so please take a moment to share your opinions with us.

Fill Out Your Survey Here

If you have any questions, don't hesitate to contact us at metabolomics.innovation@gmail.com

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metabolomics.innovation@gmail.com